EAST UPDATE 09/811,359

| L Number | Hits | Search Text | DB | Time stamp |
|---|---|---|---|---|
| 1 | 2343 | ((544/333) or (544/277)).CCLS. | USPAT; US-PGPUB | 2004/02/21 15:39 |
| 2 | 1916 | (((544/333) or (544/277)).CCLS.) and (phenyl or naphthyl) | USPAT; US-PGPUB | 2004/02/21 15:40 |
| 3 | 1861 | ((((544/333) or (544/277)).CCLS.) and (phenyl or naphthyl)) and (amino or alkoxy) | USPAT; US-PGPUB | 2004/02/21 15:41 |
| 4 | 198 | (((((544/333) or (544/277)).CCLS.) and (phenyl or naphthyl)) and (amino or alkoxy)) and ('CRF' or anxiety) | USPAT; US-PGPUB | 2004/02/21 15:41 |

09/ 811,359

Connecting via Winsock to STN

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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * *  Welcome to STN International  * * * * * * * * * *

| | | | |
|---|---|---|---|
| NEWS | 1 | | Web Page URLs for STN Seminar Schedule - N. America |
| NEWS | 2 | | "Ask CAS" for self-help around the clock |
| NEWS | 3 | SEP 09 | CA/CAplus records now contain indexing from 1907 to the present |
| NEWS | 4 | DEC 08 | INPADOC: Legal Status data reloaded |
| NEWS | 5 | SEP 29 | DISSABS now available on STN |
| NEWS | 6 | OCT 10 | PCTFULL: Two new display fields added |
| NEWS | 7 | OCT 21 | BIOSIS file reloaded and enhanced |
| NEWS | 8 | OCT 28 | BIOSIS file segment of TOXCENTER reloaded and enhanced |
| NEWS | 9 | NOV 24 | MSDS-CCOHS file reloaded |
| NEWS | 10 | DEC 08 | CABA reloaded with left truncation |
| NEWS | 11 | DEC 08 | IMS file names changed |
| NEWS | 12 | DEC 09 | Experimental property data collected by CAS now available in REGISTRY |
| NEWS | 13 | DEC 09 | STN Entry Date available for display in REGISTRY and CA/CAplus |
| NEWS | 14 | DEC 17 | DGENE: Two new display fields added |
| NEWS | 15 | DEC 18 | BIOTECHNO no longer updated |
| NEWS | 16 | DEC 19 | CROPU no longer updated; subscriber discount no longer available |
| NEWS | 17 | DEC 22 | Additional INPI reactions and pre-1907 documents added to CAS databases |
| NEWS | 18 | DEC 22 | IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields |
| NEWS | 19 | DEC 22 | ABI-INFORM now available on STN |
| NEWS | 20 | JAN 27 | Source of Registration (SR) information in REGISTRY updated and searchable |
| NEWS | 21 | JAN 27 | A new search aid, the Company Name Thesaurus, available in CA/CAplus |
| NEWS | 22 | FEB 05 | German (DE) application and patent publication number format changes |

| | |
|---|---|
| NEWS EXPRESS | DECEMBER 28 CURRENT WINDOWS VERSION IS V7.00, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003 |
| NEWS HOURS | STN Operating Hours Plus Help Desk Availability |
| NEWS INTER | General Internet Information |
| NEWS LOGIN | Welcome Banner and News Items |
| NEWS PHONE | Direct Dial and Telecommunication Network Access to STN |
| NEWS WWW | CAS World Wide Web Site (general information) |

Enter NEWS followed by the item number or name to see news on that specific topic.

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09/ 811,359

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:41:35 ON 21 FEB 2004

=> file reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 10:41:51 ON 21 FEB 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 FEB 2004 HIGHEST RN 652129-06-1
DICTIONARY FILE UPDATES: 19 FEB 2004 HIGHEST RN 652129-06-1

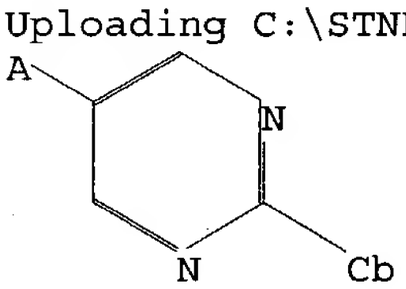
TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

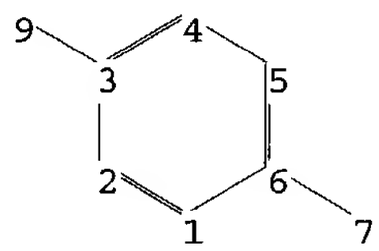
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\STNEXP4\QUERIES\09811359.str




chain nodes :
7 9
ring nodes :
1 2 3 4 5 6
chain bonds :
3-9 6-7
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
3-9
exact bonds :
6-7
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 9:CLASS
Generic attributes :

7:
Saturation : Unsaturated

Element Count :
Node 7: Limited
C,C6-12

L1 STRUCTURE UPLOADED

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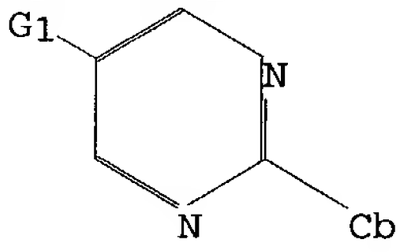


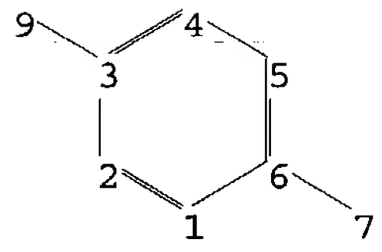


chain nodes :
7 9
ring nodes :
1 2 3 4 5 6
chain bonds :
3-9 6-7
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
3-9
exact bonds :
6-7
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
G1:O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 9:CLASS
Generic attributes :
7:
Saturation : Unsaturated

Element Count :
Node 7: Limited
C,C6-12

L2 STRUCTURE UPLOADED

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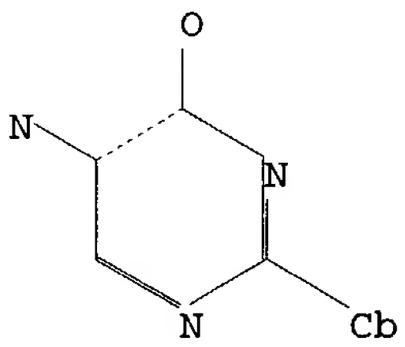


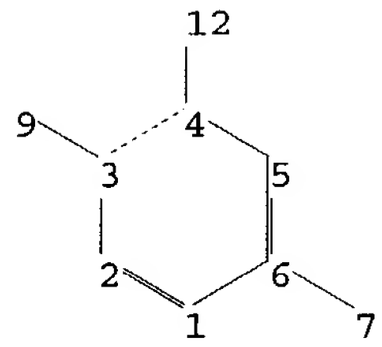


chain nodes :
7 9 12
ring nodes :
1 2 3 4 5 6
chain bonds :
3-9 4-12 6-7
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 3-9 4-5 4-12 5-6
exact bonds :
6-7
isolated ring systems :
containing 1 :

G1:O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 9:CLASS 12:CLASS
Generic attributes :
7:
Saturation : Unsaturated

Element Count :
Node 7: Limited
C,C6-12

L3 STRUCTURE UPLOADED

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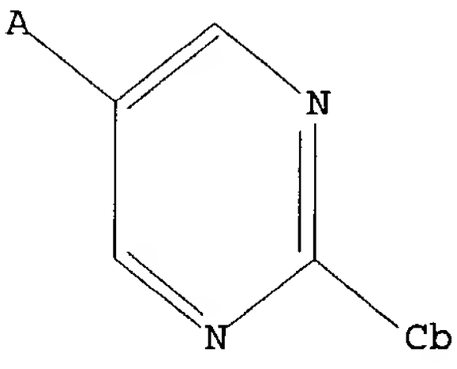
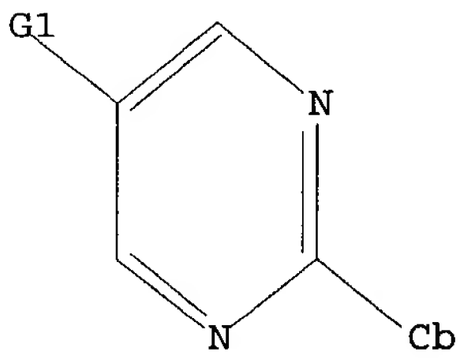
L1 HAS NO ANSWERS
L1 STR




Structure attributes must be viewed using STN Express query preparation.

=> d l2

L2 HAS NO ANSWERS
L2 STR




G1 O,N

Structure attributes must be viewed using STN Express query preparation.

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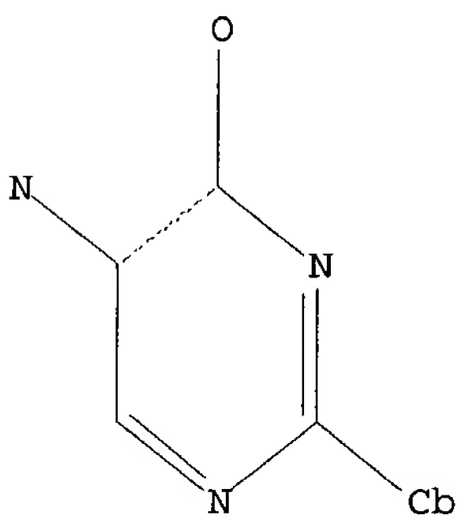
L3 STR




G1 O,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful
FULL SEARCH INITIATED 10:44:15 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 683564 TO ITERATE

58.5% PROCESSED 400000 ITERATIONS 8401 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.11

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 683564 TO 683564
PROJECTED ANSWERS: 13997 TO 14715

L4 8401 SEA SSS FUL L1

=> s l2 ful
FULL SEARCH INITIATED 10:44:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 118233 TO ITERATE

100.0% PROCESSED 118233 ITERATIONS 5166 ANSWERS
SEARCH TIME: 00.00.05

09/ 811,359

L5 5166 SEA SSS FUL L2

=> s l3 ful
FULL SEARCH INITIATED 10:44:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 33355 TO ITERATE

100.0% PROCESSED 33355 ITERATIONS 316 ANSWERS
SEARCH TIME: 00.00.02

L6 316 SEA SSS FUL L3

=> file caplus

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 467.10 | 467.31 |

FILE 'CAPLUS' ENTERED AT 10:45:05 ON 21 FEB 2004
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FILE COVERS 1907 - 21 Feb 2004 VOL 140 ISS 9
FILE LAST UPDATED: 20 Feb 2004 (20040220/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his
(FILE 'HOME' ENTERED AT 10:41:35 ON 21 FEB 2004)

FILE 'REGISTRY' ENTERED AT 10:41:51 ON 21 FEB 2004
L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 STRUCTURE UPLOADED
L4 8401 S L1 FUL
L5 5166 S L2 FUL
L6 316 S L3 FUL

FILE 'CAPLUS' ENTERED AT 10:45:05 ON 21 FEB 2004

=> s l4 or l5
1421 L4
1099 L5
L7 1933 L4 OR L5

=> s l7 not (pyridyl or pyridin? or pyrimidin? or pyrimidyl or pyridazin? or thiophen?)
42729 PYRIDYL
249931 PYRIDIN?
76023 PYRIMIDIN?
2008 PYRIMIDYL

09/ 811,359

```
          13163 PYRIDAZIN?
          57992 THIOPHEN?
L8          878 L7 NOT (PYRIDYL OR PYRIDIN? OR PYRIMIDIN? OR PYRIMIDYL OR PYRIDA
                ZIN? OR THIOPHEN?)

=> s l8 and (phenyl or naphthyl)
         309474 PHENYL
          50268 NAPHTHYL
L9           81 L8 AND (PHENYL OR NAPHTHYL)

=> s l6
L10          68 L6

=> s l9 not l10
L11          74 L9 NOT L10
```

```
=> d l10 1- ibib abs fhitstr
YOU HAVE REQUESTED DATA FROM 68 ANSWERS - CONTINUE? Y/(N):y

L10  ANSWER 1 OF 68  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         2004:20686  CAPLUS
DOCUMENT NUMBER:          140:77152
TITLE:                    Preparation of novel benzimidazole derivatives as
                          neuropeptide Y receptor antagonists
INVENTOR(S):              Otake, Norikazu; Moriya, Minoru; Ogino, Yoshio;
                          Matsuda, Kenji; Nagae, Yoshikazu; Kanatani, Akio;
                          Fukami, Takehiro
PATENT ASSIGNEE(S):       Banyu Pharmaceutical Co., Ltd., Japan
SOURCE:                   PCT Int. Appl., 171 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.         KIND  DATE          APPLICATION NO.   DATE
     ---------------    ----  --------      ---------------   --------
     WO 2004002986       A2   20040108      WO 2003-JP8161    20030626
         W:  AE, AG, AL, AM, AU, AZ, BA, BB, BR, BY, BZ, CA, CN, CO, CR, CU,
             DM, DZ, EC, GD, GH, HR, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK,
             LR, LT, LV, MA, MD, MG, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL,
             RU, SC, SG, SY, TJ, TM, TN, TT, UA, US, UZ, VC, VN, YU, ZA, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
             NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ,
             GW, ML, MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.:                    JP 2002-190978   A  20020628
OTHER SOURCE(S):          MARPAT 140:77152
GI
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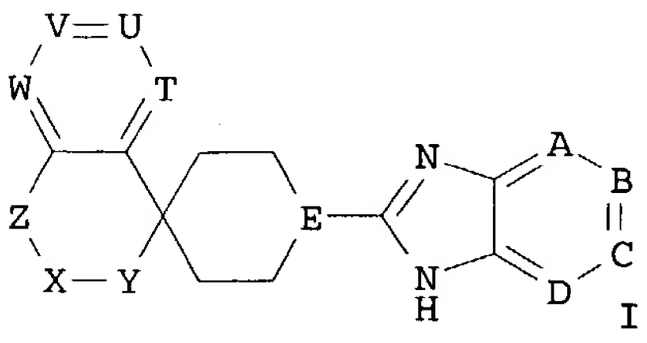
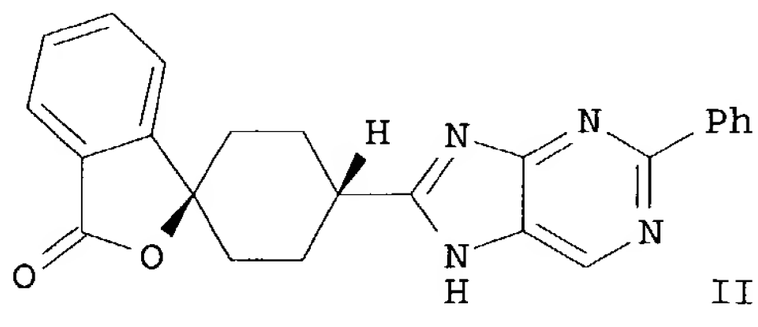



I




II

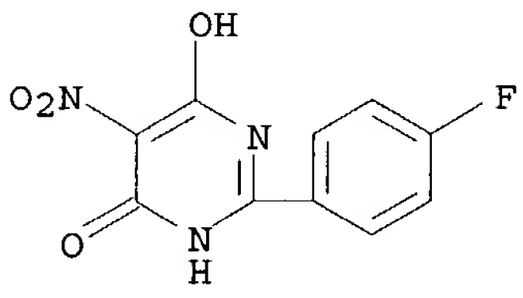
09/ 811,359

AB Benzimidazole derivs. of formula I [A, B, C, D = N, (substituted) CH; E = N, CH, C-OH; T, U, V, W = (substituted) CH, N; X = NSO2-alkyl, N-acyl, CO, etc.; Y = O, (substituted) NH, etc.; Z = (CH2)n; n = 0-1] are prepared as neuropeptide Y receptor antagonists. The compds. are useful in the treatment of bulimia, obesity or diabetes. Thus, II was prepared from trans-3'-oxospiro[cyclohexane-1,1'(3'H)-isobenzofuran]-4-carboxylic acid and 2-phenyl-4,5-diaminopyrimidine. II had IC50 of 2.2 nM in neuropeptide Y binding inhibition test. Pharmaceutical compns. containing I are described.

IT **640271-56-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzimidazole derivs. as neuropeptide Y receptor antagonists)

RN 640271-56-3 CAPLUS

CN 4(1H)-Pyrimidinone, 2-(4-fluorophenyl)-6-hydroxy-5-nitro- (9CI) (CA INDEX NAME)



L10 ANSWER 2 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:570644 CAPLUS

DOCUMENT NUMBER: 139:133575

TITLE: Preparation of bicyclic pyrimidinyl derivatives as adenosine receptor ligands

INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan

PATENT ASSIGNEE(S): OSI Pharmaceuticals Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 105 pp.
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

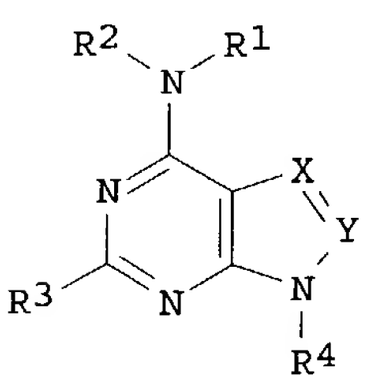
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 2003139427 | A1 | 20030724 | US 2002-227378 | 20020823 |

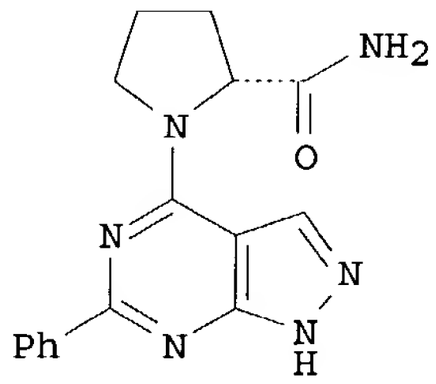
PRIORITY APPLN. INFO.: US 2002-227378 20020823

OTHER SOURCE(S): MARPAT 139:133575

GI



I



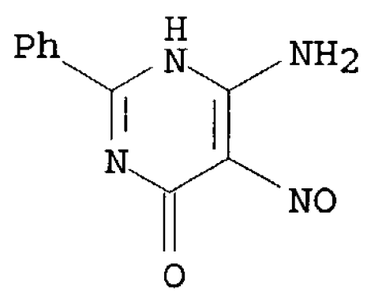
II

AB Title compds. I [Y = N, CR5 and X = N, CR6 wherein X, Y are both N or when

Y = CR5, X = N or when X = CR6, Y = N; R1-2 = H, alkoxy, aminoalkyl, etc; R3-4 = H, alkyl, aryl, alkylaryl] are prepared For instance, 3-amino-4-carbamoylpyrazole is acylated with benzoyl chloride (Pyridine, 50°, 5-6 h), cyclized to the corresponding pyrazolopyrimidine (water, K2CO3, 100°, 16 h), converted to the chloride (POCl3, 106°, 2 h) and used for reactions with various amines to give the example compds., e.g., II. II has Ki = 76.7 nM for the adenosine A1 receptor, Ki = 242.7 nM for A2a and Ki = 1480.5 nM for A2b. I are useful for the treatment of.

IT **5466-66-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bicyclic pyrazolo- imidazo- and triazolopyrimidinyl derivs. as adenosine receptor ligands)

RN 5466-66-0 CAPLUS
CN 4(1H)-Pyrimidinone, 6-amino-5-nitroso-2-phenyl- (9CI) (CA INDEX NAME)

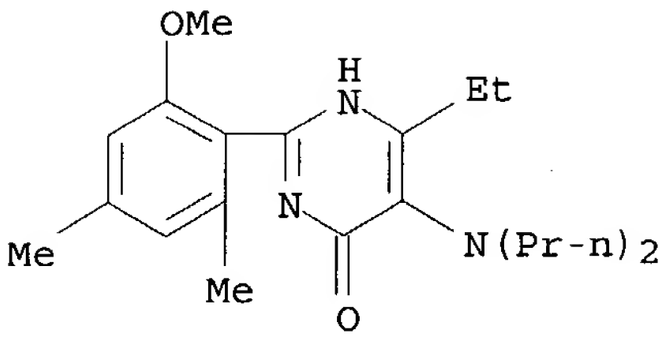


L10 ANSWER 3 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:521326 CAPLUS
DOCUMENT NUMBER: 139:239663
TITLE: 2-Aryl-3,6-dialkyl-5-dialkylaminopyrimidin-4-ones as novel CRF-1 receptor antagonists
AUTHOR(S): Hodgetts, Kevin J.; Yoon, Taeyoung; Huang, Jianhua; Gulianello, Michael; Kieltyka, Andrzej; Primus, Renee; Brodbeck, Robbin; De Lombaert, Stephane; Doller, Dario
CORPORATE SOURCE: Neurogen Corporation, Branford, CT, 06405, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(15), 2497-2500
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The discovery, synthesis and structure-activity studies of a novel series of 2-arylpyrimidin-4-ones as CRF-1 receptor antagonists is described. These compds. are structurally simple and display appropriate phys. properties for CNS agents.

IT **391936-44-0P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation, phys. properties, and biol. activity of 2-aryl-3,6-dialkyl-5-dialkylaminopyrimidin-4-ones as novel CRF-1 receptor antagonists)

RN 391936-44-0 CAPLUS
CN 4(1H)-Pyrimidinone, 5-(dipropylamino)-6-ethyl-2-(2-methoxy-4,6-dimethylphenyl)- (9CI) (CA INDEX NAME)

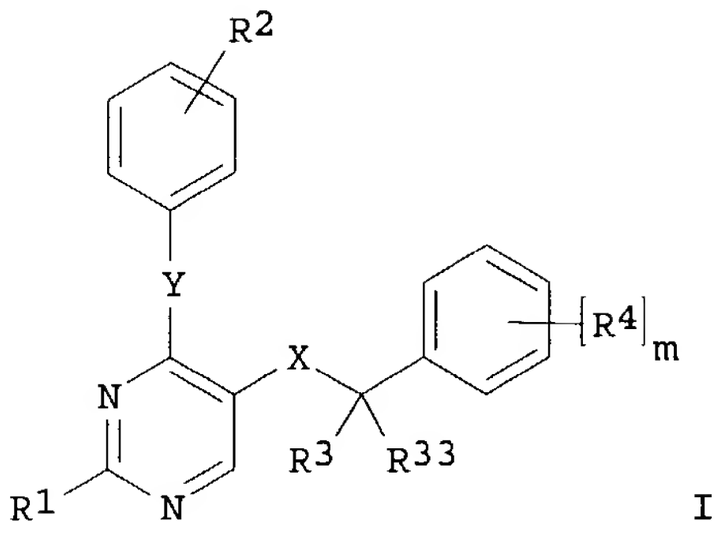



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:408655 CAPLUS
DOCUMENT NUMBER: 137:6189
TITLE: Preparation of pyrimidine derivatives as NK1 antagonists
INVENTOR(S): Stadler, Heinz
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2002042280 | A2 | 20020530 | WO 2001-EP13084 | 20011113 |
| WO 2002042280 | A3 | 20020822 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 2002099207 | A1 | 20020725 | US 2001-977586 | 20011015 |
| AU 2002027921 | A5 | 20020603 | AU 2002-27921 | 20011113 |
| EP 1339698 | A2 | 20030903 | EP 2001-989463 | 20011113 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| BR 2001015480 | A | 20031021 | BR 2001-15480 | 20011113 |
| NO 2003002291 | A | 20030521 | NO 2003-2291 | 20030521 |

PRIORITY APPLN. INFO.: EP 2000-125529 A 20001122
WO 2001-EP13084 W 20011113
OTHER SOURCE(S): MARPAT 137:6189
GI



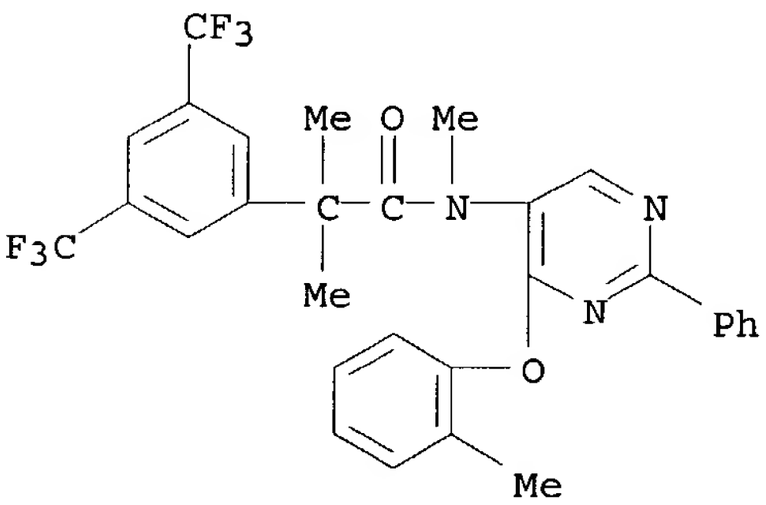
I

AB The title compds. [I; R1 = alkyl, alkoxy, pyridinyl, pyrimidinyl, etc.; R2 = H, alkyl, alkoxy, halo, CF3; R3, R33 = H, alkyl; R4 = halo, CF3, alkoxy; R5 = H, alkyl; X = CONR, NRCO; Y = O, S, SO2, NR; m = 0-2] which have a good affinity to the NK1 receptor and therefore are suitable in the treatment of diseases, related to this receptor, were prepared and formulated. Thus, reacting 4-chloro-2-methylsulfanylpyrimidine-5-carboxylic acid Et ester with o-cresol in the presence of Cs2CO3 in MeCN (99%) followed by saponification (47%), and amidation of the resulting acid with [3,5-bis(trifluoromethyl)benzyl]methylamine (96%) afforded I [R1 = SMe; R2 = 2-Me; R3, R33 = H; R4 = 3,5-(CF3)2; Y = O; X = CONMe] which showed pKi of 7.38 against NK-1 receptor binding.

IT **432521-49-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidine derivs. as NK1 antagonists)

RN 432521-49-8 CAPLUS

CN Benzeneacetamide, N,α,α-trimethyl-N-[4-(2-methylphenoxy)-2-phenyl-5-pyrimidinyl]-3,5-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 5 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

| | |
|---|---|
| ACCESSION NUMBER: | 2002:72057 CAPLUS |
| DOCUMENT NUMBER: | 136:134771 |
| TITLE: | Preparation of 5-substituted 2-aryl-4-pyrimidinones as selective modulators of CRF 1 receptors |
| INVENTOR(S): | Hodgetts, Kevin J.; Doller, Dario |
| PATENT ASSIGNEE(S): | Neurogen Corporation, USA |
| SOURCE: | PCT Int. Appl., 75 pp.<br>CODEN: PIXXD2 |
| DOCUMENT TYPE: | Patent |
| LANGUAGE: | English |
| FAMILY ACC. NUM. COUNT: | 1 |

09/ 811,359

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2002006242 | A2 | 20020124 | WO 2001-US22513 | 20010718 |
| WO 2002006242 | A3 | 20020718 | | |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

| | | | | |
|---|---|---|---|---|
| US 2002052387 | A1 | 20020502 | US 2001-908444 | 20010718 |
| EP 1301490 | A2 | 20030416 | EP 2001-958986 | 20010718 |

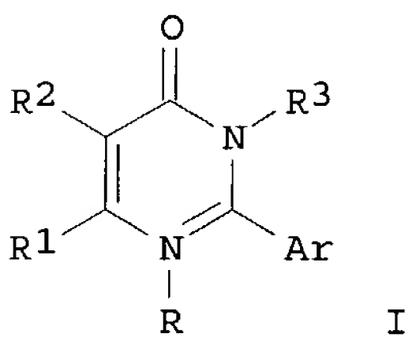
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

| | | | | |
|---|---|---|---|---|
| JP 2004504302 | T2 | 20040212 | JP 2002-512146 | 20010718 |

PRIORITY APPLN. INFO.: US 2000-219703P P 20000718
WO 2001-US22513 W 20010718

OTHER SOURCE(S): MARPAT 136:134771

GI



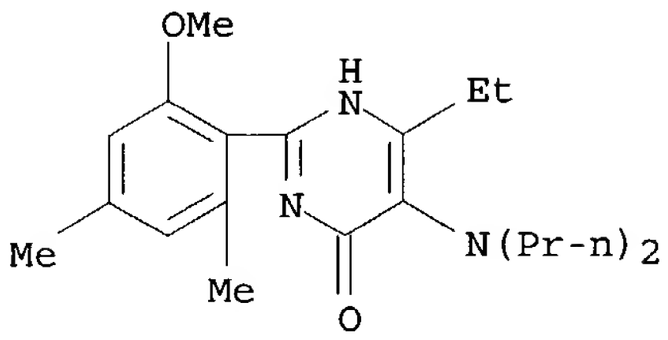
I

AB The title compds. [I; Ar = (un)substituted carbocyclic aryl, heteroaryl; R = O, Me, absent; R1 = H, halo, CN, etc.; R2 = alkyl, alkoxy, cycloalkyl, etc.; R3 = H, alkyl, alkoxy, (di)alkylamino, etc.; provided that R1 is not H, alkyl, or CF3 when R2 = H, alkyl, alkenyl] that act as selective modulators of CRF 1 receptors, and therefore are useful in the treatment of a number of CNS and peripheral disorders, particularly stress, anxiety, depression, cardiovascular disorders, and eating disorders, were prepared E.g., a multi-step synthesis of I [Ar = 2-MeO-4,6-Me2C6H2; R1 = Me; R2 = NPr2; R3 = Me] was given. The exemplified compds. I showed IC50 of ≤ 4 μM in assay for CRF1 receptor binding activity. Compds. I are also useful as probes for the localization of CRF receptors and as stds. in assays for CRF receptor binding. Methods of using the compds. I in receptor localization studies are given.

IT **391936-44-0P**
RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 5-substituted 2-aryl-4-pyrimidinones as selective modulators of CRF 1 receptors)

RN 391936-44-0 CAPLUS

CN 4(1H)-Pyrimidinone, 5-(dipropylamino)-6-ethyl-2-(2-methoxy-4,6-dimethylphenyl)- (9CI) (CA INDEX NAME)




L10 ANSWER 6 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:693291 CAPLUS
DOCUMENT NUMBER: 135:242241
TITLE: 5-Substituted arylpyrimidines as selective modulators of CRF receptors
INVENTOR(S): Yoon, Taeyound; Delombaert, Stephane; Hodgetts, Kevin; Doller, Dario
PATENT ASSIGNEE(S): Neurogen Corporation, USA
SOURCE: PCT Int. Appl., 83 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001068614 | A2 | 20010920 | WO 2001-US8321 | 20010316 |
| WO 2001068614 | A3 | 20020606 | | |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 2002072521 | A1 | 20020613 | US 2001-811359 | 20010316 |
| EP 1233949 | A2 | 20020828 | EP 2001-916687 | 20010316 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| JP 2003527377 | T2 | 20030916 | JP 2001-567707 | 20010316 |

PRIORITY APPLN. INFO.:
US 2000-189774P P 20000316
US 2000-206454P P 20000522
WO 2001-US8321 W 20010316

OTHER SOURCE(S): MARPAT 135:242241

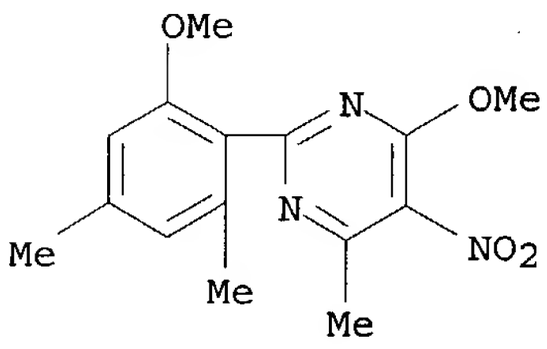
AB 2-Ar-4-R1-5-R2-6-R3pyrimidines (I, or a pharmaceutically acceptable salt thereof) are provided that can act as selective modulators of CRF receptors. In I: Ar is Ph, 1- or 2-naphthyl, each of which is mono, di, or trisubstituted or mono, di, or trisubstituted heteroaryl having from .apprx.5 to .apprx.7 ring members and 1 to .apprx.4 heteroatoms in the ring, the heteroatoms independently = N, O and S; R1 and R3 independently = H, halogen, cyano, nitro, alkyl, alkenyl, alkynyl, alkoxy, (cycloalkyl)alkyl, alkylthio, alkylsulfinyl, alkylsulfonyl, or mono- or dialkylcarboxamide, with the proviso that R1 and R3 are not both H; and R2 is alkyl, alkenyl, alkynyl, alkoxy, aminoalkyl, mono or dialkylamino, alkylthio, alkylsulfinyl, alkylsulfonyl, mono or dialkylcarboxamide, carbocyclic aryl or heteroaryl having from 1 to 3 rings, and 3 to 8 ring members in each ring and 1 to .apprx.3 heteroatoms. These compds. are useful in the treatment of a number of CNS and peripheral disorders, particularly stress, anxiety, depression, cardiovascular disorders, and

eating disorders. Methods of treatment of such disorders as well as packaged pharmaceutical compns. are also provided. Compds. of the invention are also useful as probes for the localization of CRF receptors and as stds. in assays for CRF receptor binding. Methods of using the compds. in receptor localization studies are given. Compds. of the invention do not exhibit activity as sodium ion channel blockers. They do exhibit in vitro t1/2 values of greater than 10 min and less than 4 h. MDCK toxicity was also measured. Six example prepns. are included, but the methods of preparation are not claimed.

IT **360576-58-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of 5-substituted arylpyrimidines as selective modulators of CRF receptors)

RN 360576-58-5 CAPLUS

CN Pyrimidine, 4-methoxy-2-(2-methoxy-4,6-dimethylphenyl)-6-methyl-5-nitro- (9CI) (CA INDEX NAME)




L10 ANSWER 7 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:489401 CAPLUS
DOCUMENT NUMBER: 135:92657
TITLE: Preparation of 2-(2-alkoxy-5-sulfonylphenyl)-3H-imidazo[1,5-a][1,3,5]triazin-4-ones as inhibitors of cGMP metabolizing phosphodiesterases
INVENTOR(S): Niewoehner, Ulrich; Haning, Helmut; Lampe, Thomas; Es-Sayed, Mazen; Schmidt, Gunter; Bischoff, Erwin; Dembowsky, Klaus; Perzborn, Elisabeth; Schlemmer, Karl-Heinz
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 73 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2001047928 | A2 | 20010705 | WO 2000-EP12597 | 20001212 |
| WO 2001047928 | A3 | 20020516 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| DE 19962928 | A1 | 20010628 | DE 1999-19962928 | 19991224 |
| DE 10003323 | A1 | 20010802 | DE 2000-10003323 | 20000127 |

09/ 811,359

| | | | | |
|---|---|---|---|---|
| EP 1244673 | A2 | 20021002 | EP 2000-993611 | 20001212 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| BR 2000017043 | A | 20030107 | BR 2000-17043 | 20001212 |
| JP 2003519150 | T2 | 20030617 | JP 2001-549398 | 20001212 |
| US 2003195210 | A1 | 20031016 | US 2002-168194 | 20021104 |

PRIORITY APPLN. INFO.: DE 1999-19962928 A 19991224
DE 2000-10003323 A 20000127
WO 2000-EP12597 W 20001212

OTHER SOURCE(S): MARPAT 135:92657
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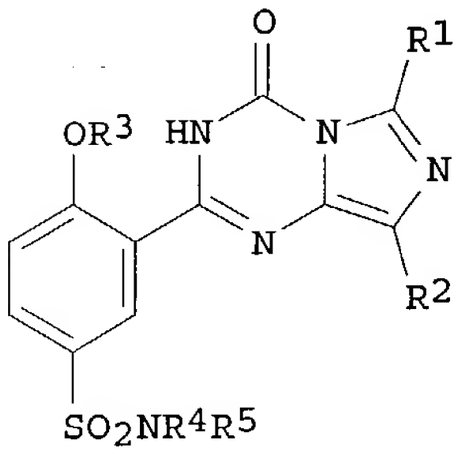
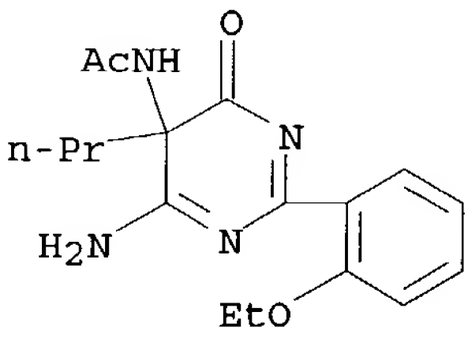


I

AB Title compds. [I; R1 = alkyl; R2 = alkyl, cycloalkyl; R3 = H, alkyl; R4, R5 = H, alkoxy, OH, (substituted) alkyl] were prepared as inhibitors of cGMP metabolizing phosphodiesterases (no data). Thus, 4-ethoxy-3-(6-methyl-4-oxo-8-propyl-3,4-dihydroimidazo[1,5-a][1,3,5]triazin-2-yl)benzenesulfonyl chloride (preparation given) in CH2Cl2 was stirred with N-(3,4-dimethoxyphenylethyl)-N-methylamine for 2 h at room temperature to give 98% N-[2-(3,4-dimethoxyphenyl)ethyl]-4-ethoxy-N-methyl-3-(6-methyl-4-oxo-8-propyl-3,4-dihydroimidazo[1,5-a][1,3,5]triazin-2-yl)benzenesulfonamide.

IT **346605-61-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of alkoxysulfonylphenylimidazotriazinones as inhibitors of cGMP metabolizing phosphodiesterases)

RN 346605-61-6 CAPLUS
CN Acetamide, N-[6-amino-2-(2-ethoxyphenyl)-4,5-dihydro-4-oxo-5-propyl-5-pyrimidinyl]- (9CI) (CA INDEX NAME)



L10 ANSWER 8 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:479151 CAPLUS
DOCUMENT NUMBER: 135:76905
TITLE: Preparation of imidazotriazinones as cGMP PDE inhibitors
INVENTOR(S): Niewoehner, Ulrich; Haning, Helmut; Lampe, Thomas;

Es-Sayed, Mazen; Schmidt, Gunter; Bischoff, Erwin; Dembowsky, Klaus; Perzborn, Elisabeth; Schlemmer, Karl-Heinz
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 38 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 19962928 | A1 | 20010628 | DE 1999-19962928 | 19991224 |
| WO 2001047928 | A2 | 20010705 | WO 2000-EP12597 | 20001212 |
| WO 2001047928 | A3 | 20020516 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1244673 | A2 | 20021002 | EP 2000-993611 | 20001212 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| BR 2000017043 | A | 20030107 | BR 2000-17043 | 20001212 |
| ZA 2002004457 | A | 20030604 | ZA 2002-4457 | 20001212 |
| JP 2003519150 | T2 | 20030617 | JP 2001-549398 | 20001212 |

PRIORITY APPLN. INFO.: DE 1999-19962928 A 19991224
DE 2000-10003323 A 20000127
WO 2000-EP12597 W 20001212

OTHER SOURCE(S): MARPAT 135:76905
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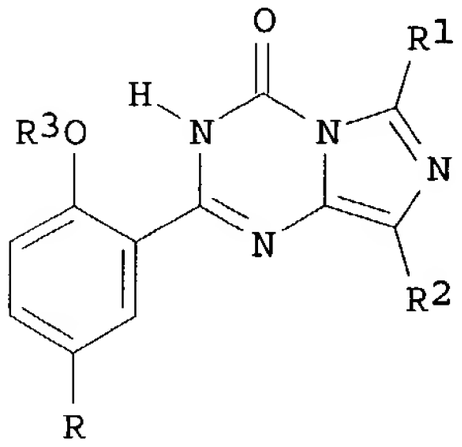

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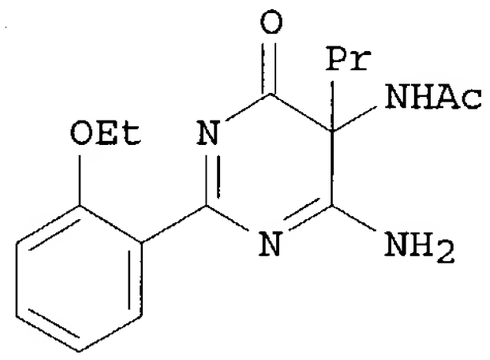


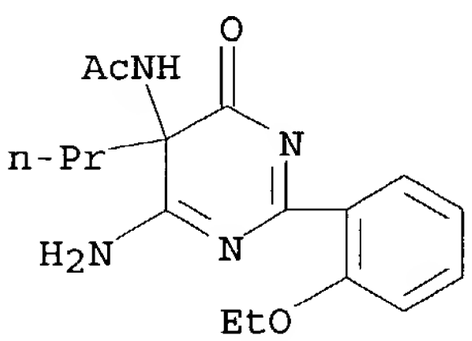
II

AB Title compds. [I; R1 = alkyl; R2 = (cyclo)alkyl; R3 = H or alkyl; R4,R5 = H, (un)substituted alkyl, alkoxy, etc.; NR4R5 = heterocyclyl] were prepared as cGMP PDE inhibitors (no data). Thus, 2-(EtO)C6H4C(:NH)NH2.HCl was cyclocondensed with PrC(CN)(NHAc)CO2Et (preparation each given) to give pyrimidinone II which was treated with Me3SiCl and the product refluxed with NH(SiMe3)3 to give, after chlorosulfonation, I (R = SO2R6, R1 = Me, R2 = Pr, R3 = Et)(III; R6 = Cl). The latter was amidated by 1-(2-hydroxyethyl)piperazine to give III [R6 = 4-(2-hydroxyethyl)-1-piperazinyl].
IT **346605-61-6P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of imidazotriazinones as cGMP PDE inhibitors)

RN 346605-61-6 CAPLUS

CN Acetamide, N-[6-amino-2-(2-ethoxyphenyl)-4,5-dihydro-4-oxo-5-propyl-5-pyrimidinyl]- (9CI) (CA INDEX NAME)




L10 ANSWER 9 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:279454 CAPLUS

DOCUMENT NUMBER: 134:295831

TITLE: Preparation of 2-(2-alkoxy-5-heterocyclylsulfonylphenyl)purin-6-ones as phosphodiesterase inhibitors

INVENTOR(S): Maw, Graham Nigel; Rawson, David James

PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.

SOURCE: Eur. Pat. Appl., 44 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

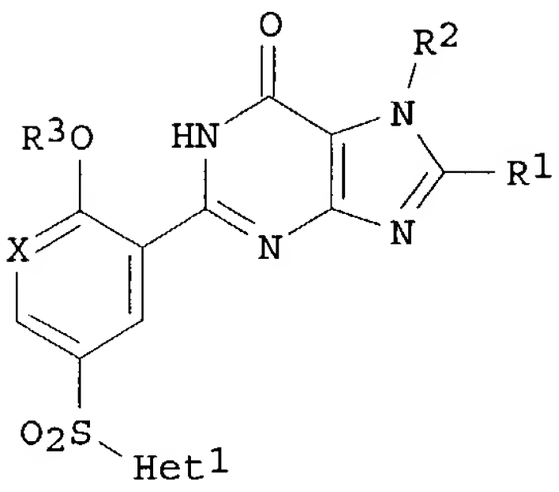
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 1092718 | A1 | 20010418 | EP 2000-308644 | 20001002 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| US 6440982 | B1 | 20020827 | US 2000-650848 | 20000829 |
| JP 2001114782 | A2 | 20010424 | JP 2000-310665 | 20001011 |
| BR 2000004786 | A | 20010522 | BR 2000-4786 | 20001011 |
| JP 2003128673 | A2 | 20030508 | JP 2002-224638 | 20001011 |
| US 2003004173 | A1 | 20030102 | US 2002-189655 | 20020703 |
| US 6593332 | B2 | 20030715 | | |
| US 2003013727 | A1 | 20030116 | US 2002-189680 | 20020703 |
| US 6586439 | B2 | 20030701 | | |

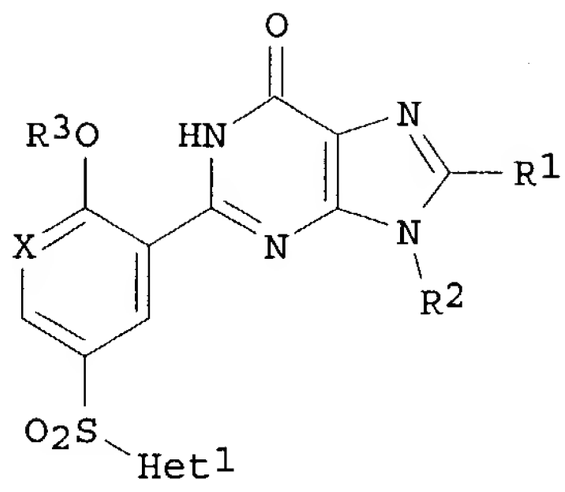
PRIORITY APPLN. INFO.:
GB 1999-24020 A 19991011
US 2000-650848 A3 20000829
JP 2000-310665 A3 20001011

OTHER SOURCE(S): MARPAT 134:295831

GI



I



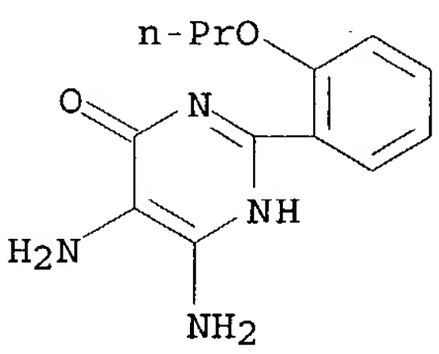
II

AB The title compds. [I or II; X = CH, N; R1 = H, CN, aryl, etc.; R2 = H, aryl, alkyl, etc.; R3 = H, (un)substituted alkyl; Het1 = 4-12 membered heterocyclyl which contains at least one N atom and, optionally, one or more further heteroatoms selected from N, O, and/or S], useful in the curative and prophylactic treatment of medical conditions for which inhibition of a cyclic guanosine 3',5'-monophosphate phosphodiesterase (e.g. cGMP PDE5) is desired (such as male erectile dysfunction), were prepared and formulated. E.g., 3-step synthesis of II [X = CH; R1 = H; R2, R3 = Pr; Het1 = 4-(pyridin-2-yl)piperazin-1-yl] which showed 100% PDE5 inhibition at 10 nM, was given.

IT **57075-34-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 2-(2-alkoxy-5-heterocyclylsulfonylphenyl)purin-6-ones as phosphodiesterase inhibitors)

RN 57075-34-0 CAPLUS

CN 4(1H)-Pyrimidinone, 5,6-diamino-2-(2-propoxyphenyl)- (9CI) (CA INDEX NAME)

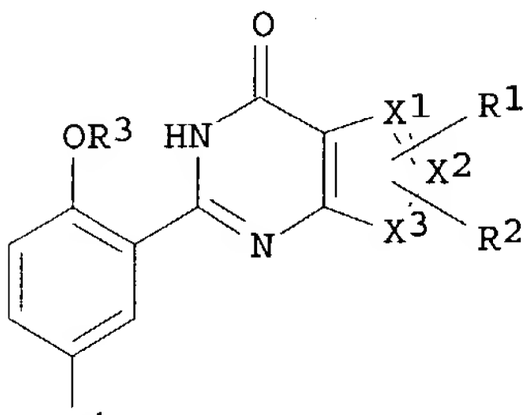


REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

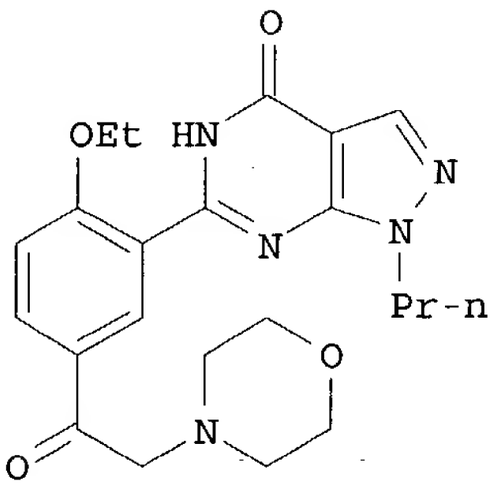
L10 ANSWER 10 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:179819 CAPLUS
DOCUMENT NUMBER: 134:222726
TITLE: Preparation of phenyl purinone derivatives for the treatment of precancerous lesions
INVENTOR(S): Piazza, Gary A.; Pamukcu, Rifat
PATENT ASSIGNEE(S): Cell Pathways, Inc., USA
SOURCE: U.S., 31 pp., Cont. of U. S. Ser. No. 472,804.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|

US 6200980 B1 20010313 US 1997-842854 19970417
PRIORITY APPLN. INFO.: US 1995-472804 A1 19950607
OTHER SOURCE(S): MARPAT 134:222726
GI



I

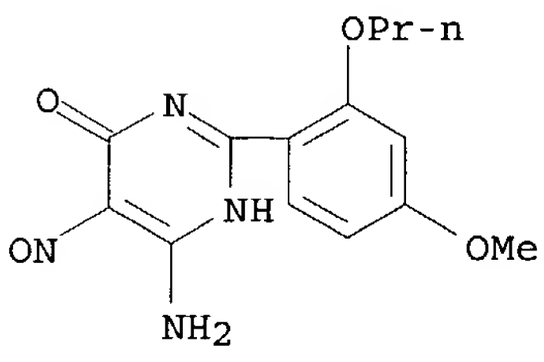


II

AB Title compds. (I) [wherein R1 = H, (fluoro)alkyl, or cycloalkyl; R2 = H, (fluoro)alkyl, or cycloalkylalkyl; R3 = (fluoro)alkyl, cycloalkyl(alkyl), alkenyl or alkynyl; R4 = halo or (un)substituted alkyl, alkenyl, alkanoyl, carbamoyl, carboxy, amino, sulfamoylamino, Ph, pyridyl, or imidazoyl, etc.; X1-X3 = independently N or C with the proviso that at least 2 of X1-X3 = N] were prepared for inhibiting the growth of neoplastic cells. For example, the 4H-pyrazolo[3,4-d]pyrimidin-4-one (II) was formed in a multi-step synthesis involving amidation of 5-amino-1-propylpyrazole-4-carboxamide with 2-ethoxybenzoyl chloride (74%), cyclization using aqueous NaOH (89%), acetylation with bromoacetyl bromide in the presence of AlCl3 (92%), and addition of morpholine in K2CO3 and MeCN (85%). In a cell growth inhibition assay examining the effects of I on human colon carcinoma cells, administration of 40 μM of 2-(2-propoxyphenyl)-8-azapurin-6-one resulted in 30% apoptotic cells and 2% necrosis compared to 7% and 5%, resp., for the control. Pharmaceutical compns. for oral and parenteral administration of I are also included.

IT **127979-83-3P**, 2-(4-Methoxy-2-propoxyphenyl)-4-amino-5-nitrosopyrimidin-6-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of Ph purinone derivs. for treatment of precancerous lesions)

RN 127979-83-3 CAPLUS
CN 4(1H)-Pyrimidinone, 6-amino-2-(4-methoxy-2-propoxyphenyl)-5-nitroso- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 137 THERE ARE 137 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

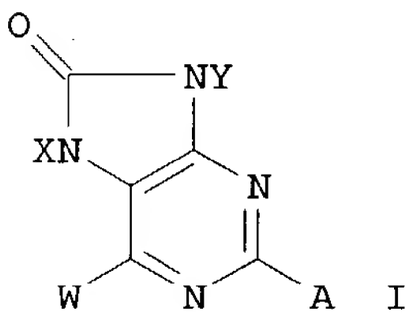
L10 ANSWER 11 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:124174 CAPLUS

09/ 811,359

DOCUMENT NUMBER: 134:173047
TITLE: Pharmaceuticals containing 2-aryl-8-oxodihydropurines for anxiolytics and antidepressants
INVENTOR(S): Murata, Akiya; Masumoto, Kaoru; Kondo, Masanori; Furukawa, Kiyoshi; Oka, Makoto
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 36 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 2001048882 | A2 | 20010220 | JP 2000-165263 | 20000602 |

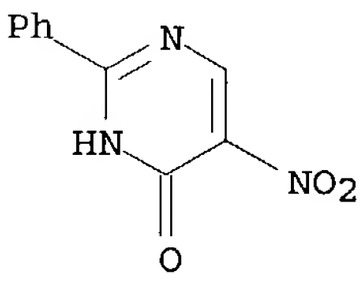
PRIORITY APPLN. INFO.: JP 1999-154830 A 19990602
OTHER SOURCE(S): MARPAT 134:173047
GI



I

AB The pharmaceuticals contain dihydropurines I [W = H, lower alkyl, halo, lower alkoxy, amino, etc.; X = H, lower alkyl, (cycloalkyl)alkyl, phenylalkyl, CHR3CONR1R2, etc.; R1 = lower alkyl, alkenyl, cycloalkyl, etc.; R2 = lower alkyl, cycloalkyl, Ph, etc.; R3 = H, lower alkyl, hydroxyalkyl; Y = H, lower alkyl, cycloalkyl, (cycloalkyl)alkyl, lower alkenyl, CHR3CONR1R2, etc.; A = (un)substituted Ph, heteroaryl; ≥1 group selected from X, Y is CHR3CONR1R2] or pharmaceutically acceptable acid salts. 7,9-Dihydro-9-methyl-2-phenyl-8H-purin-8-one (7.0 g) was reacted with 8.3 g 2-bromo-N-ethyl-N-phenylacetamide in the presence of NaH in DMF at room temperature for 3 h to give 10.3 g N-ethyl-8,9-dihydro-9-methyl-8-oxo-2-phenyl-N-phenyl-7H-purine-7-acetamide showing good antidepressant activity in rats.

IT **3749-46-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(pharmaceuticals containing aryloxodihydropurines for anxiolytics and antidepressants)
RN 3749-46-0 CAPLUS
CN 4(1H)-Pyrimidinone, 5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 12 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:861681 CAPLUS

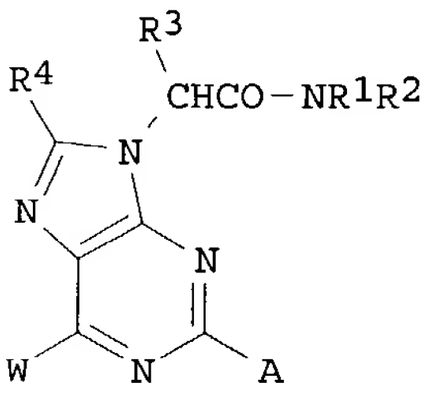
09/ 811,359

DOCUMENT NUMBER: 134:17498
TITLE: Preparation of 2-arylpurine-9-acetamide derivatives having selective action on peripheral benzodiazepine receptor, process for the preparation thereof, medicinal compositions containing the same and intermediates of the derivatives
INVENTOR(S): Murata, Teruya; Kondo, Katsunori; Masumoto, Kaoru; Kohayakawa, Hitoshi; Furukawa, Kiyoshi
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 78 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000073306 | A1 | 20001207 | WO 2000-JP3374 | 20000526 |
| JP 2003146987 | A2 | 20030521 | JP 1999-150878 | 19990531 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: JP 1999-150878 A 19990531
OTHER SOURCE(S): MARPAT 134:17498
GI




W N A I

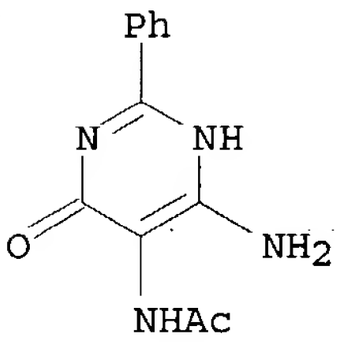
AB The title 2-arylpurine-9-acetamide derivs. represented by general formula (I; R1 is lower alkyl, cycloalkyl, cycloalkylated lower alkyl, or the like; R2 is lower alkyl, substituted or unsubstituted Ph, or the like; R3 is hydrogen or the like; R4 is hydrogen, lower alkyl, cycloalkyl, halogeno, lower alkoxy, or the like; A is substituted or unsubstituted Ph or the like; W is hydrogen, lower alkyl, halogeno, lower alkoxy, lower alkylthio, lower alkanoyl, or the like) or pharmaceutically acceptable acid addition salts thereof are prepared as well as pharmaceutical compns. containing them. These compds. selectively act on peripheral benzodiazepine receptor BZω3 receptor and are useful as therapeutic and preventive drugs for central nervous system diseases such as anxiety-related diseases, depression and epilepsy. Thus, a mixture of 2-(5-amino-2-phenyl-4-pyrimidinylamino)-N-methyl-N-phenylacetamide and DMF was heated at 180° with stirring for 2 h to give N-methyl-N-phenyl-2-phenyl-9H-purine-9-acetamide (II). II and N-methyl-N-phenyl-8-chloro-2-phenyl-9H-purine-9-acetamide inhibited the binding of [3H]4'-chlorodiazepam to BZω3 receptor prepared from rat kidney with IC50 of 0.88 and 0.23 nM,

resp.

IT **310408-58-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-arylpurine-9-acetamide derivs. having selective action on peripheral benzodiazepine receptor as drugs)

RN 310408-58-3 CAPLUS

CN Acetamide, N-(6-amino-1,4-dihydro-4-oxo-2-phenyl-5-pyrimidinyl)- (9CI) (CA INDEX NAME)

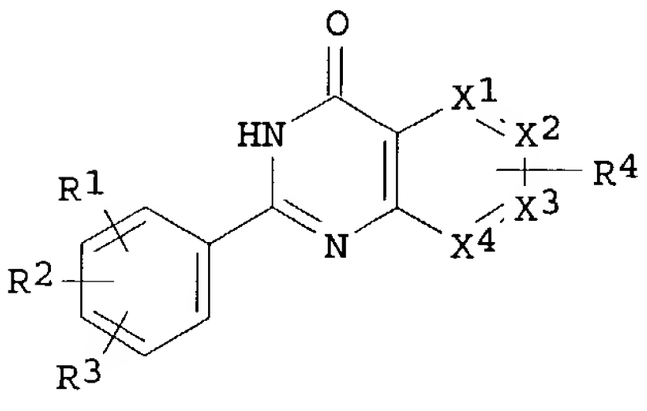



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 13 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:304315 CAPLUS
DOCUMENT NUMBER: 132:321870
TITLE: Preparation of pyridopyrimidinones, pyrimidopyrimidinones, pyrimidotriazinones, and related compounds for the treatment of precancerous lesions.
INVENTOR(S): Piazza, Gary A.; Pamukcu, Rifat
PATENT ASSIGNEE(S): Cell Pathways, Inc., USA
SOURCE: U.S., 19 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 6060477 | A | 20000509 | US 1995-484002 | 19950607 |
| US 6391885 | B1 | 20020521 | US 2000-564196 | 20000504 |

PRIORITY APPLN. INFO.: US 1995-484002 A3 19950607
OTHER SOURCE(S): MARPAT 132:321870
GI




I

AB A method for treating precancerous lesions comprises administration of title compds. [I; R1-R3 = H, halo, alkyl, alkoxy, alkenyl, alkenyloxy,

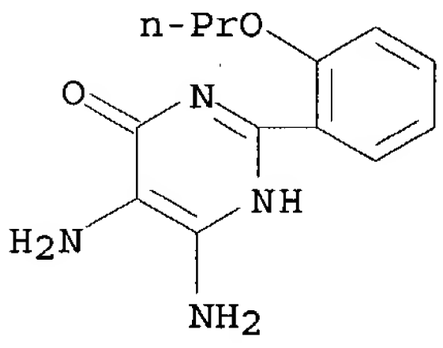
alkylthio, alkylamino, cyano, acylamino, etc.; R4 = H, alkyl, alkoxy, Ph, OH, halo, acylamino, aminoacyl, 5-tetrazolyl, cyano, etc.; X1-X4 = N, C; ≥1 of X1-X4 = N, ≥1 of X1-X4 = C] (no data). Thus, 2-propoxybenzoyl chloride in MeCN was added to a mixture of 2-aminonicotinamide and Et3N in MeCN at 0° followed by 1.5 h stirring and standing overnight to give 2-(2-propoxybenzamido)nicotinamide. This was refluxed 30 min. with pyridine in aqueous NaOH to give 2-(2-propoxyphenyl)pyrido[2,3-d]pyrimid-4(3H)-one. A capsule formulation containing the latter is given.

IT **127979-73-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyridopyrimidinones, pyrimidopyrimidinones, pyrimidotriazinones, and related compds. for the treatment of precancerous lesions)

RN 127979-73-1 CAPLUS
CN 4(1H)-Pyrimidinone, 5,6-diamino-2-(2-propoxyphenyl)-, sulfate (1:1) (9CI) (CA INDEX NAME)

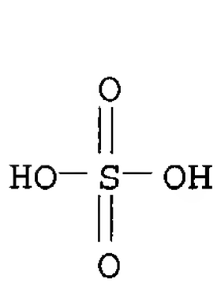
CM 1

CRN 57075-34-0
CMF C13 H16 N4 O2




CM 2

CRN 7664-93-9
CMF H2 O4 S




REFERENCE COUNT: 126 THERE ARE 126 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 14 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:511159 CAPLUS
DOCUMENT NUMBER: 131:157709
TITLE: Preparation of bicyclic pyridine and pyrimidine derivatives as neuropeptide Y receptor antagonists
INVENTOR(S): Norman, Mark H.; Chen, Ning; Han, Nianhe; Liu, Longbin; Hurt, Clarence R.; Fotsch, Christopher H.; Jenkins, Tracy J.; Moreno, Ofir A.
PATENT ASSIGNEE(S): Amgen Inc., USA
SOURCE: PCT Int. Appl., 469 pp.
CODEN: PIXXD2

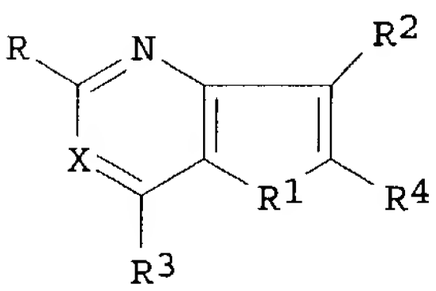
09/ 811,359

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9940091 | A1 | 19990812 | WO 1999-US2500 | 19990205 |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 6187777 | B1 | 20010213 | US 1999-246775 | 19990204 |
| CA 2319275 | AA | 19990812 | CA 1999-2319275 | 19990205 |
| AU 9926590 | A1 | 19990823 | AU 1999-26590 | 19990205 |
| AU 747920 | B2 | 20020530 | | |
| EP 1054887 | A1 | 20001129 | EP 1999-906756 | 19990205 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| JP 2003502272 | T2 | 20030121 | JP 2000-530520 | 19990205 |
| ZA 9900967 | A | 19990806 | ZA 1999-967 | 19990208 |
| US 6583154 | B1 | 20030624 | US 2000-640263 | 20000816 |

| PRIORITY APPLN. INFO.: | | | |
|---|---|---|---|
| | US 1998-73927P | P | 19980206 |
| | US 1998-73981P | P | 19980206 |
| | US 1998-93482P | P | 19980720 |
| | US 1998-93577P | P | 19980720 |
| | US 1999-246775 | A | 19990204 |
| | WO 1999-US2500 | W | 19990205 |

OTHER SOURCE(S): MARPAT 131:157709
GI



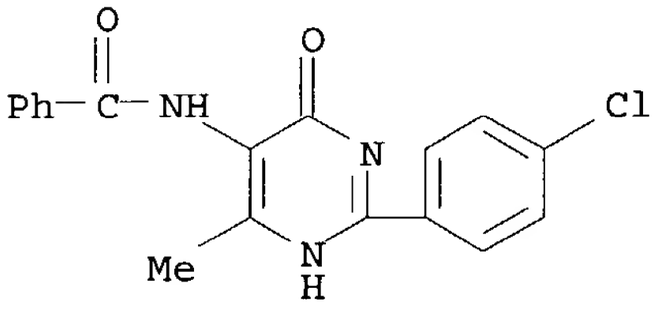

I

AB Title compds. [I; R = H, CH3, (CH3)2CH, SCH3, CH3CH2, NH2, CF3, NHCOC6H5, cyclopropyl, CH2OH, (CH3)2CH2CH2, N(CH3)2, OCH3, NHCH3, NH(CH2)4NH2; R1 = NH, S, NCH3, O; R2 = H, COCH3, C6H5, CH3, CH3CH2; R3 = NH2, CH3, NHC6H5, N(CH2CH3)2, (CH3CH2)N(CH2)3CH3, (CH3)N(CH2)2NHCH3, N(CH3)CH(CH3)CH(Ph)OH, (CH3CH2)NCH2C(CH3):CH2, NHCH2CF3, NHCH2CH2C6H5, NH(CH2)3OCH2CH3, 4-ClC6H4, 4-CH3OC6H5, 2-thienyl, 1-pyrrolidinyl, 1-piperidinyl, 4-morpholinyl, 1-piperazinyl, 3-pyridyl; R4 = C6H5, 4-CH3C6H4, 4-ClC6H4, (CH3)3C, 4-FC6H4, 3-HOC6H4, 2-pyridyl, cyclohexyl, 2-furyl, 2-FC6H4 2-thienyl, 1-adamantyl, CH3, 4-CH3OC6H4; X = N, CH; etc.], pharmaceutical acceptable salts, ester, solvate, and N-oxide are prepared and tested as neuropeptide Y receptor antagonists in the modulation of feeding behavior, obesity, diabetes, cancer, inflammatory disorders, depression, stress related disorders, Alzheimer's disease and other disease conditions. Thus, the title compound I (R = CH3; R1 = NH; X = N; R2 = H; R3 = N(CH2CH3)2; R4 = C6H5) was prepared

IT **237435-23-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation of pyrrolopyridine and pyrrolopyrimidine derivs. as neuropeptide Y receptor antagonists)

RN 237435-23-3 CAPLUS
CN Benzamide, N-[2-(4-chlorophenyl)-1,4-dihydro-6-methyl-4-oxo-5-pyrimidinyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

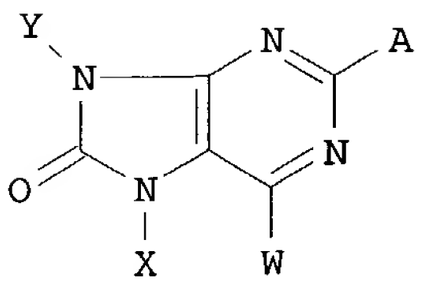
L10 ANSWER 15 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:375547 CAPLUS
DOCUMENT NUMBER: 131:31952
TITLE: Preparation of 2-aryl-8-oxodihydropurine derivatives as anxiolytics
INVENTOR(S): Murata, Teruya; Masumoto, Kaoru; Kondo, Katsunori; Furukawa, Kiyoshi; Oka, Makoto
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 86 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9928320 | A1 | 19990610 | WO 1998-JP5320 | 19981126 |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| ZA 9810490 | A | 19990520 | ZA 1998-10490 | 19981117 |
| TW 502034 | B | 20020911 | TW 1998-87119571 | 19981125 |
| CA 2312885 | AA | 19990610 | CA 1998-2312885 | 19981126 |
| AU 9912604 | A1 | 19990616 | AU 1999-12604 | 19981126 |
| AU 744014 | B2 | 20020214 | | |
| EP 1036794 | A1 | 20000920 | EP 1998-955937 | 19981126 |
| EP 1036794 | B1 | 20030827 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| BR 9815140 | A | 20001010 | BR 1998-15140 | 19981126 |
| NZ 504457 | A | 20011221 | NZ 1998-504457 | 19981126 |
| AT 248169 | E | 20030915 | AT 1998-955937 | 19981126 |
| RU 2223272 | C2 | 20040210 | RU 2000-117278 | 19981126 |
| US 6372740 | B1 | 20020416 | US 2000-555490 | 20000601 |
| NO 2000002835 | A | 20000724 | NO 2000-2835 | 20000602 |

PRIORITY APPLN. INFO.: JP 1997-350000 A 19971203
WO 1998-JP5320 W 19981126

09/ 811,359

GI



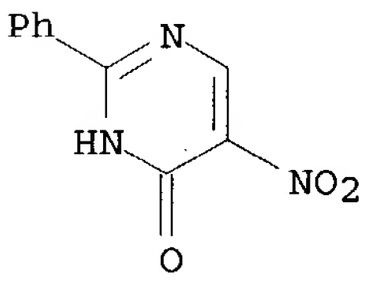
I

AB Title compds. I (W = H, alkyl, halo, alkoxy, amino, alkylamino, Ph, substituted Ph; X = H, alkyl, alkenyl, carbamoyl, etc.; Y = H, alkyl, cycloalkyl, alkenyl, etc.; A = Ph, substituted Ph, heteroaryl, etc.) and their pharmaceutically acceptable salts, useful as anxiolytics (no data), were prepared Thus, reaction of 7,9-dihydro-9-methyl-2-phenyl-8H-purin-8-one with 2-bromo-N-ethyl-N-phenyl-acetamide in DMF in the presence of NaH at room temperature for 3 h gave N-ethyl-8,9-dihydro-9-methyl-8-oxo-2-phenyl-N-phenyl-7H-purine-7-acetamide. Formulations containing I were given.

IT **3749-46-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2-aryl-8-oxodihydropurine derivs. as anxiolytics)

RN 3749-46-0 CAPLUS

CN 4(1H)-Pyrimidinone, 5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 16 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:314282 CAPLUS

DOCUMENT NUMBER: 129:54385

TITLE: Preparation of acetic acid amide derivatives as drugs

INVENTOR(S): Murata, Akiya; Hino, Katsuhiko; Furukawa, Kiyoshi; Oka, Makoto; Ito, Mari

PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 44 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

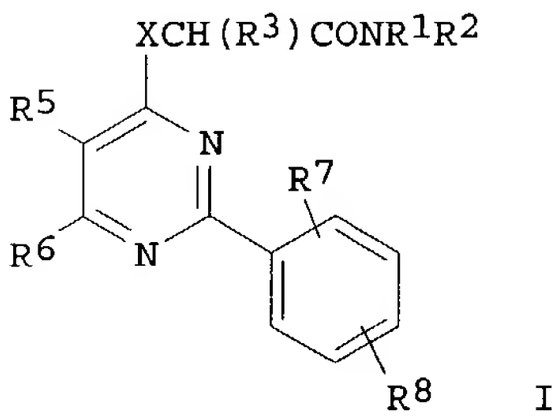
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 10130150 | A2 | 19980519 | JP 1997-257573 | 19970905 |

PRIORITY APPLN. INFO.: JP 1996-257704 19960905

OTHER SOURCE(S): MARPAT 129:54385

GI



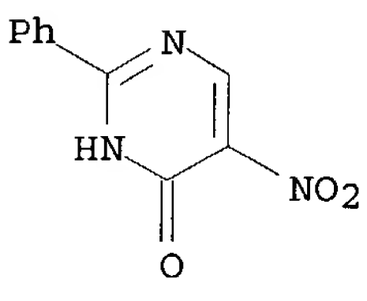
I

AB The title compds. [I; X = O, NR4; R1 = H, (un)substituted lower alkyl or alkenyl, etc.; R2 = cycloalkyl, lower alkyl, (un)substituted Ph, etc.; R3 = H, alkyl, hydroxyalkyl, etc.; R4 = H, alkyl, or combine with R3 and N to form a pyrrolidine or piperidine; R5 = H, lower alkyl or alkenyl, hydroxyalkyl, CF3, etc.; R6 = H, lower alkyl, CF3, etc.; R7 = H, halo, lower alkyl, etc.; R8 = H, halo, lower alkoxy, etc.] are prepared I, possessing affinity toward the benzodiazepine receptor, are useful for prevention and treatment of melancholia, insecure related diseases, central nervous system diseases, and immunity inflammation diseases. Thus, 4-chloro-5,6-dimethyl-2-phenylpyrimidine was reacted with 2-amino-N,N-dipropylacetamide in the presence of Et3N to give I (R1 = R2 = n-Pr, R3 = R7 = R8 = H, R5 = R6 = Me, X = NH), which showed IC50 of 3.10 nM with abenzodiazepine receptor (BZω3) when tested with rat. A formulation containing I was also prepared

IT **3749-46-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of acetic acid amide derivs. as drugs)

RN 3749-46-0 CAPLUS

CN 4(1H)-Pyrimidinone, 5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 17 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:407610 CAPLUS

DOCUMENT NUMBER: 127:121691

TITLE: Synthesis of 4,6-disubstituted and 4,5,6-trisubstituted 2-phenylpyrimidines and their affinity towards A1 adenosine receptors

AUTHOR(S): Biagi, Giuliana; Giorgi, Irene; Livi, Oreste; Scartoni, Valerio; Lucacchini, Antonio

CORPORATE SOURCE: Dip. Scienze Farmaceutiche, Univ. Pisa, Pisa, 56126, Italy

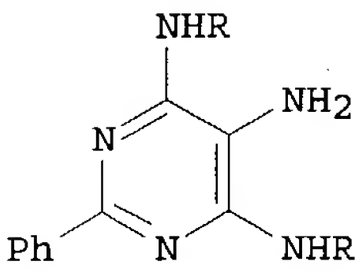
SOURCE: Farmaco (1997), 52(1), 61-65
CODEN: FRMCE8; ISSN: 0014-827X

PUBLISHER: Societa Chimica Italiana

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



@ HCl

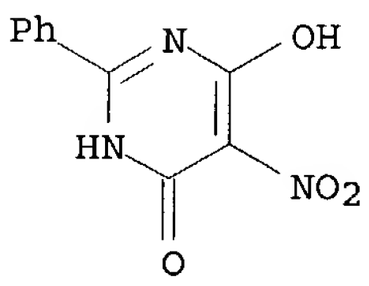
I

AB The preparation and assay of the title compds., e.g., I (R = cyclohexyl, pentyl), are reported. The results support our hypothesis about the possibility that mols. characterized by great flexibility, such as 2-phenyl-4,5,6-triaminopyrimidines, can better interact with the receptor sites than rigid mols. such as 2,6,9-trisubstituted 8-azaadenines. The relatively low activity shown by pyrimidine derivs. demonstrated the importance of the bicyclic aromatic system in 8-azaadenines and adenines for a favorable interaction with the A1 adenosine receptors.

IT **68905-99-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 4,6-disubstituted and 4,5,6-trisubstituted 2-phenylpyrimidines and their A1 adenosine receptor affinity)

RN 68905-99-7 CAPLUS

CN 4(1H)-Pyrimidinone, 6-hydroxy-5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 18 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:753799 CAPLUS

DOCUMENT NUMBER: 126:18884

TITLE: Preparation and formulation of pyrimidine derivatives as agents with effect on the peripheral benzodiazepine receptors

INVENTOR(S): Murata, Teruya; Hino, Katsuhiko; Furukawa, Kiyoshi; Oka, Makoto; Itoh, Mari

PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 110 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9632383 | A1 | 19961017 | WO 1996-JP977 | 19960410 |
| W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK | | | | |
| RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML | | | | |
| IL 117659 | A1 | 20001206 | IL 1996-117659 | 19960326 |
| ZA 9602438 | A | 19961001 | ZA 1996-2438 | 19960327 |

| | | | | |
|---|---|---|---|---|
| CA 2218033 | AA | 19961017 | CA 1996-2218033 | 19960410 |
| AU 9652874 | A1 | 19961030 | AU 1996-52874 | 19960410 |
| AU 694647 | B2 | 19980723 | | |
| EP 826673 | A1 | 19980304 | EP 1996-909327 | 19960410 |
| EP 826673 | B1 | 20021120 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI | | | | |
| CN 1186487 | A | 19980701 | CN 1996-194408 | 19960410 |
| CN 1094929 | B | 20021127 | | |
| BR 9604894 | A | 19980714 | BR 1996-4894 | 19960410 |
| RU 2160256 | C2 | 20001210 | RU 1997-118591 | 19960410 |
| SK 281840 | B6 | 20010806 | SK 1997-1374 | 19960410 |
| CZ 289093 | B6 | 20011017 | CZ 1997-3223 | 19960410 |
| RO 117532 | B1 | 20020430 | RO 1997-1858 | 19960410 |
| AT 228113 | E | 20021215 | AT 1996-909327 | 19960410 |
| PT 826673 | T | 20030228 | PT 1996-96909327 | 19960410 |
| ES 2187644 | T3 | 20030616 | ES 1996-909327 | 19960410 |
| TW 450963 | B | 20010821 | TW 1996-85104372 | 19960412 |
| NO 9704685 | A | 19971212 | NO 1997-4685 | 19971010 |
| US 5972946 | A | 19991026 | US 1997-930604 | 19971014 |

PRIORITY APPLN. INFO.: JP 1995-113937 A 19950413
WO 1996-JP977 W 19960410

OTHER SOURCE(S): MARPAT 126:18884

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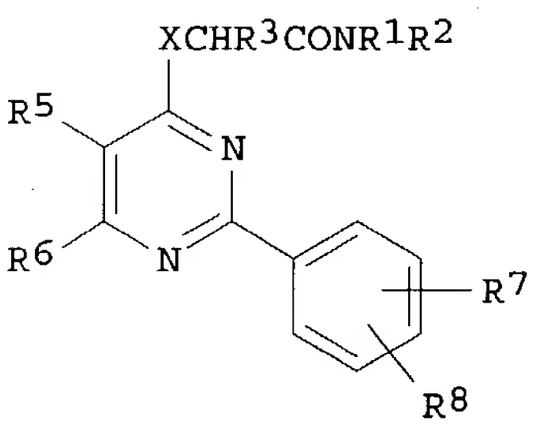


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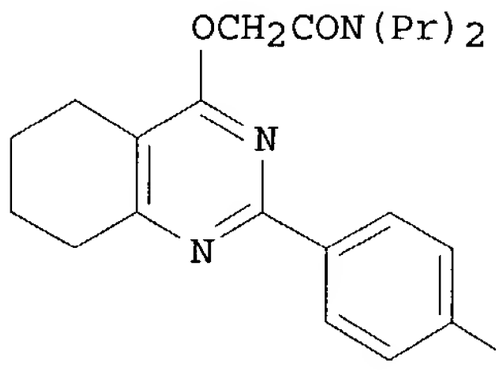
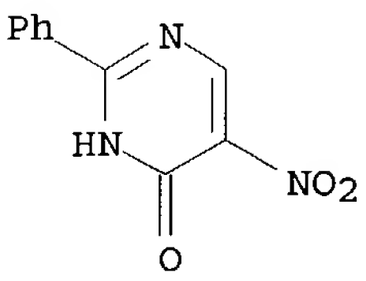



II

AB The title compds. I [X represents O or NR4; R1 represents H, lower alkyl, lower alkenyl or cycloalkyl(lower)alkyl; R2 represents lower alkyl, cycloalkyl, optionally substituted Ph, etc.; R3 represents H, lower alkyl or hydroxy(lower)alkyl; R4 represents H, lower alkyl, etc.; R5 represents hydroxy(lower)alkyl, etc.; R6 represents H, lower alkyl, CF3 or optionally substituted Ph, or R5 and R6 together form (CH2)n; n = 3 - 6; R7 represents H, halogeno, lower alkyl, lower alkoxy, CF3, OH, NH2, etc.; and R8 represents H, halogeno, lower alkyl or lower alkoxy] are prepared In an in vitro test for affinity for the peripheral benzodiazepine receptors, the title compound II in vitro showed IC50 of 0.89 nM.

IT **3749-46-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidine derivs. as agents with effect on peripheral benzodiazepine receptors)

RN 3749-46-0 CAPLUS
CN 4(1H)-Pyrimidinone, 5-nitro-2-phenyl- (9CI) (CA INDEX NAME)

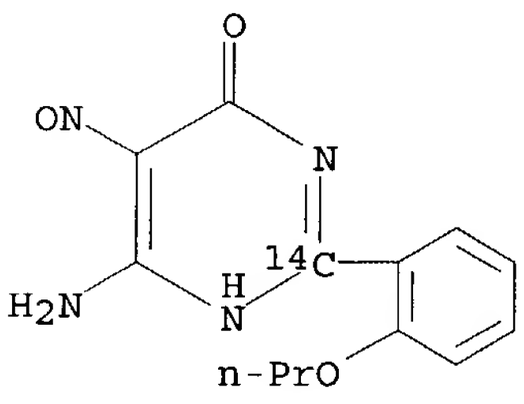


L10 ANSWER 19 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:777454 CAPLUS
DOCUMENT NUMBER: 123:340001
TITLE: Carbon-14 labeled nitrogen heterocycles. The syntheses of these phosphodiesterase inhibitors
AUTHOR(S): Lawrie, Kenneth W. M.; Novelli, Christine E. A.; Saunders, David; Coastes, William J.
CORPORATE SOURCE: New Froniters Sci. Park, SmithKline Beecham Pharm. Res. Dev. Synth. Isotope Chem. Dep., Essex, CM19 5AW, UK
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (1995), 36(9), 891-8
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The syntheses of three heterocyclic phosphodiesterase inhibitors are described from a common radiolabeled precursor, namely 2-propoxybenzo[cyano-14C]nitrile. Conversion of the nitrile to the corresponding Me ketone or amidine allows elaboration of the heterocycles radiolabeled within the ring systems. The target compds. were [14C]-labeled 7-(cyclopropylamino)-2-(2-propoxyphenyl)pyrimido[4,5-d]pyrimidin-4(1H)-one (SF&K 97992) and 1,7-dihydro-2-(2-propoxyphenyl)-6H-purin-6-one (SF&K 96231).

IT **170703-44-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of [14C]-labeled purinone and pyrimido[4,5-d]pyrimidinone)

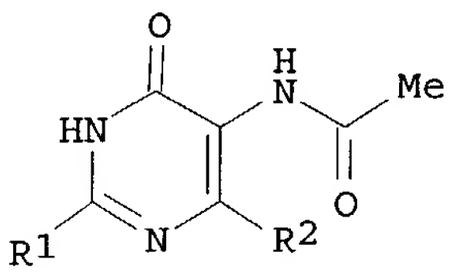
RN 170703-44-3 CAPLUS
CN 4(1H)-Pyrimidinone-2-14C, 6-amino-5-nitroso-2-(2-propoxyphenyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 20 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:691725 CAPLUS
DOCUMENT NUMBER: 123:111733
TITLE: Synthesis of 2,6-disubstituted 5-aminopyrimidine-4-ones from 2,6-disubstituted 5-acetylpyrimidin-4-one oximes through Beckmann rearrangement
AUTHOR(S): Yamamoto, Yutaka; Ogawa, Yoshitaka
CORPORATE SOURCE: Tohoku Coll. Pharm., Komatsushima 4-chome, Sendai,

09/ 811,359

SOURCE: 981, Japan
Yakugaku Zasshi (1995), 115(3), 256-60
CODEN: YKKZAJ; ISSN: 0031-6903
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
OTHER SOURCE(S): CASREACT 123:111733
GI

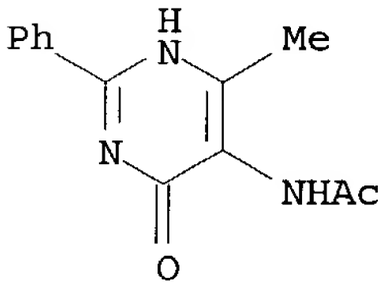


I

AB 2,6-Disubstituted 5-acetylpyrimidin-4-one oximes were heated in formic acid under reflux to undergo Beckmann rearrangement, giving 2,6-disubstituted 5-acetylaminopyrimidin-4-ones (I; R1, R2 = Ph, Me; p-ClC6H4, Me; Ph, p-MeC6H4; Ph, 3-pyridyl) in good yields.

IT **72168-63-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of disubstituted 5-aminopyrimidineones from disubstituted 5-acetylpyrimidinone oximes through Beckmann rearrangement)

RN 72168-63-9 CAPLUS
CN Acetamide, N-(1,4-dihydro-6-methyl-4-oxo-2-phenyl-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 21 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:655817 CAPLUS
DOCUMENT NUMBER: 121:255817
TITLE: Process for preparation of cycloalkyl- and azacycloalkylpyrrolopyrimidines useful as GABAa receptor ligands
INVENTOR(S): Thurkauf, Andrew; Hutchison, Alan; Singh, Vinod
PATENT ASSIGNEE(S): Neurogen Corp., USA
SOURCE: Braz. Pedido PI, 101 pp.
CODEN: BPXXDX
DOCUMENT TYPE: Patent
LANGUAGE: Portuguese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| BR 9201262 | A | 19931013 | BR 1992-1262 | 19920408 |
| RU 2055077 | C1 | 19960227 | RU 1992-5011467 | 19920406 |
| RO 109942 | B1 | 19950728 | RO 1992-478 | 19920407 |

09/ 811,359

PRIORITY APPLN. INFO.: SU 1992-5011467 A 19920406
BR 1992-1262 19920408

OTHER SOURCE(S): MARPAT 121:255817

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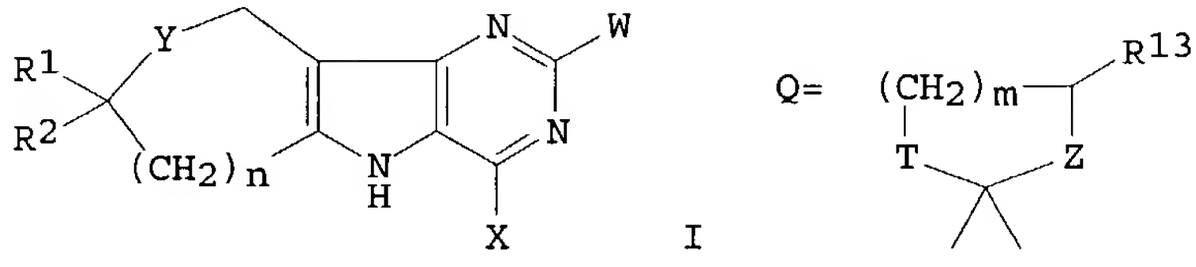


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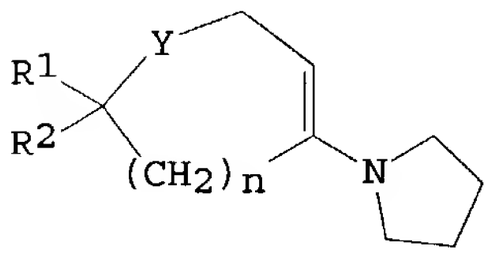


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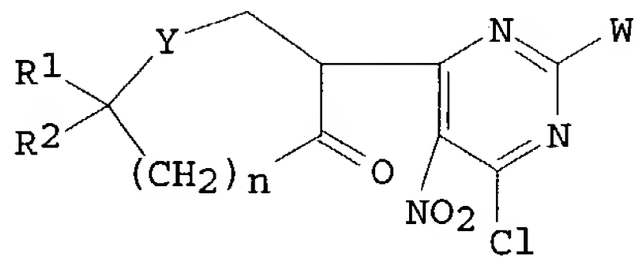
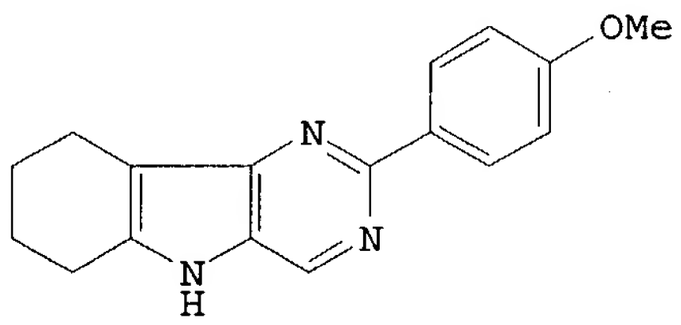



III



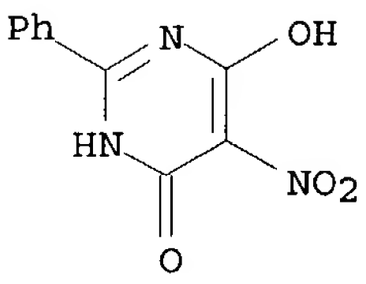

IV

AB Title compds. I [n = 0, 1, 2; R1, R2 = H, alkyl; X = H, OH; W = (un)substituted Ph, thienyl, pyridyl; Y = NR3, CO, CR6(OR5), CR6(COR5), CR6(CO2R5), CR6(OCOR5), CR5R6, CR6(CONR7R8), CR6[(CH2)nNR7R8], CR6(NR9CO2R10), CR6[C(OH)R11R12], cyclic group Q; R3 = H, alkyl, Ph, pyridyl, phenylalkyl, (di)(alkyl)aminoalkyl, (un)substituted 1-indanyl, 4-(thio)chromanyl, or 1,2,3,4-tetrahydro-1-naphthyl, COR4, SO2R4; R4 = alkyl, Ph, phenylalkyl, phenylalkoxy; R5, R8, R9, R10, R13, R14 = H, alkyl, Ph, pyridyl, phenylalkyl; R6, R7 = H, alkyl; or NR7R8 = morpholino, piperidino, pyrrolidino, or N-alkylpiperazino; R11, R12 = alkyl, Ph, phenylalkyl; m = 0, 1, 2; Z = CH2, O, NR14, CHCONR14 (sic); T = CH2, O] were prepared (77 examples). I are highly selective agonists, antagonists, inverse agonists, or prodrugs for cerebral GABAa receptors, and are useful for diagnosis or treatment of anxiety, convulsions, sleep disturbances, or benzodiazepine overdose, or for improving activity (sic). Preparation of I involves 5 steps: (1) reaction of dialkyl malonates with arylamidines WC(:NH)NH2 to give 2-aryl-4,6-dihydroxypyrimidines; (2) nitration of these in the 5-position; (3) treatment of the resultant arylnitrodihydroxypyrimidines with POCl3 to give 2-aryl-5-nitro-4,6-dichloropyrimidines; (4) coupling of these with cyclic pyrrolidine enamines II to give 4-substituted 5-nitro-6-chloropyrimidines III; and (5) catalytic hydrogenation of III with cyclization. In tests for binding to rat cortical GABAa receptors in vitro, 12 selected I had IC50 of 0.009-1.00 μM, e.g., 0.039 μM for IV, a preferred compound

IT **68905-99-7P**, 4(1H)-Pyrimidinone, 6-hydroxy-5-nitro-2-phenyl-
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of GABAergic cycloalkyl- and azacycloalkylpyrrolopyrimidines)

RN 68905-99-7 CAPLUS

CN 4(1H)-Pyrimidinone, 6-hydroxy-5-nitro-2-phenyl- (9CI) (CA INDEX NAME)




L10 ANSWER 22 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:655782 CAPLUS
DOCUMENT NUMBER: 121:255782
TITLE: Preparation of aryl heterocyclyl pyrimidines as GABA brain receptor ligands
INVENTOR(S): Thurkauf, Andrew; Hutchison, Alan
PATENT ASSIGNEE(S): Neurogen Corp., USA
SOURCE: U.S., 17 pp. Cont. of U.S. Ser. No. 865,129, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 5326868 | A | 19940705 | US 1993-106193 | 19930812 |
| WO 9425463 | A1 | 19941110 | WO 1993-US3917 | 19930430 |
| W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, RO, RU, SD, SE, SK, UA, US, UZ, VN | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| AU 9341174 | A1 | 19941121 | AU 1993-41174 | 19930430 |
| US 5463054 | A | 19951031 | US 1994-269667 | 19940701 |

PRIORITY APPLN. INFO.: US 1992-865129 19920408
WO 1993-US3917 19930430
US 1993-106193 19930812

OTHER SOURCE(S): MARPAT 121:255782

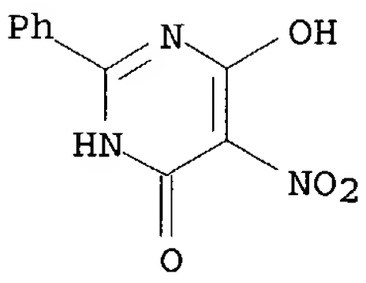
GI For diagram(s), see printed CA Issue.

AB Title compds. I (X = H, halo, HO; W = (substituted) aryl; A, B, C, D, E = C or N substituted with H or various organic and inorg. substituents; R3, R4 = organic and inorg. substituents), are prepared 2-(2-Fluoro-4-methoxyphenyl)6,7,8,9-tetrahydro-5H-indolo[3,2-d]pyrimidine and Pd black in mesitylene was stirred at 230° to give the title compound 2-(2-fluoro-4-methoxyphenyl)5H-indolo[3,2-d]pyrimidine. I demonstrated GABAa receptor activity.

IT **68905-99-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aryl heterocyclyl pyrimidines as GABA brain receptor ligands)

RN 68905-99-7 CAPLUS

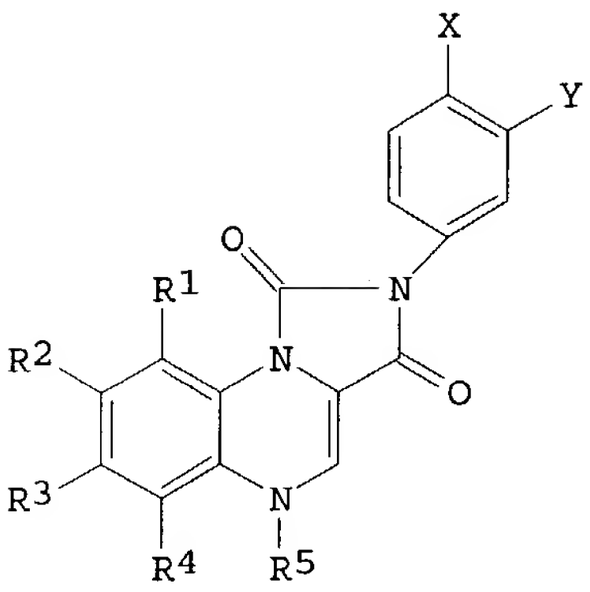
CN 4(1H)-Pyrimidinone, 6-hydroxy-5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



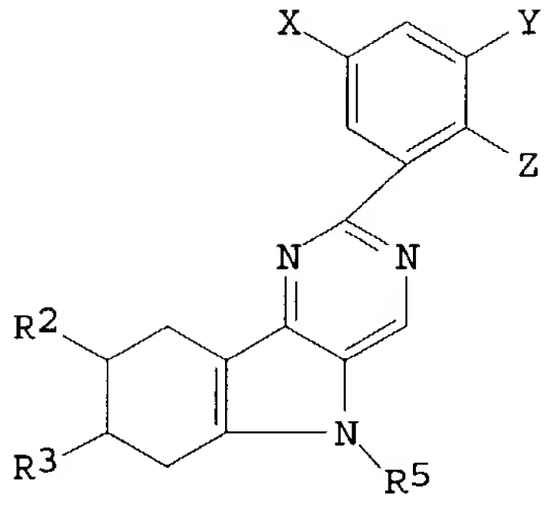

L10 ANSWER 23 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:95809 CAPLUS
DOCUMENT NUMBER: 120:95809
TITLE: Novel GABAa receptor subtypes and methods for screening drug compounds using imidazoquinoxalines and pyrrolopyrimidines to bind to GABAa receptor subtypes
INVENTOR(S): Shaw, Kenneth; Hutchison, Alan; Thurkauf, Andrew; Tallman, John
PATENT ASSIGNEE(S): Neurogen Corp., USA
SOURCE: PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9322681 | A1 | 19931111 | WO 1993-US3920 | 19930430 |
| W: AT, AU, BB, BG, BR, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, RO, RU, SD, SE, SK, UA, US, VN | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| US 5597920 | A | 19970128 | US 1992-876050 | 19920430 |
| AU 9341177 | A1 | 19931129 | AU 1993-41177 | 19930430 |
| AU 691470 | B2 | 19980521 | | |
| EP 639275 | A1 | 19950222 | EP 1993-910819 | 19930430 |
| EP 639275 | B1 | 19970917 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE | | | | |
| JP 08500333 | T2 | 19960116 | JP 1993-519445 | 19930430 |
| AT 158414 | E | 19971015 | AT 1993-910819 | 19930430 |
| ES 2110090 | T3 | 19980201 | ES 1993-910819 | 19930430 |
| US 5688654 | A | 19971118 | US 1994-331501 | 19941028 |

PRIORITY APPLN. INFO.: US 1992-876050 19920430
WO 1993-US3920 19930430
OTHER SOURCE(S): MARPAT 120:95809
GI



I



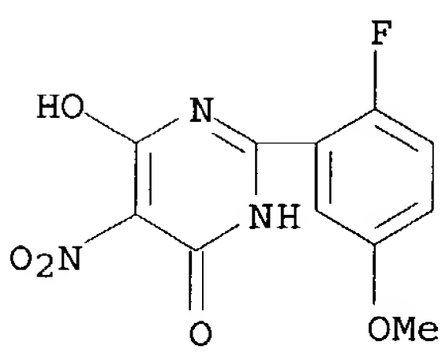
II

AB Imidazoquinoxalines I and pyrrolopyrimidines II (R1-R4, X, Y = H, halo, alkyl, alkoxy; R5 = H, lower alkyl; Z = H, F) bind selectively to a novel subtype of the GABAa binding site. Selective interaction of ligands at this unique receptor population results in pharmacol. specificity which may lead to superior anxiolytics, cognition enhancers, anticonvulsants, and hypnotics. Such drugs may be screened by measuring their competition with 3H- or I isotope-labeled I or II for binding to these GABAa receptors. Thus, I (R1-R5, Y = H; X = OEt) (III) bound with high affinity (Ki 0.5 nM) to rat cortical GABAa receptors. III-3H was prepared by reaction of 2-nitrophenyl isocyanate, 3-bromo-4-ethoxyaniline, and ClCH2COCl, reduction of the NO2 group with Fe powder to cyclize, further bromination in positions 6 and 8, and tritiation with T2 over Pd/C.

IT **152336-01-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)

RN 152336-01-1 CAPLUS

CN 4(1H)-Pyrimidinone, 2-(2-fluoro-5-methoxyphenyl)-6-hydroxy-5-nitro- (9CI) (CA INDEX NAME)



L10 ANSWER 24 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:582837 CAPLUS
DOCUMENT NUMBER: 119:182837
TITLE: Arylazopyrimidines as dichroic dyes for liquid crystals
AUTHOR(S): Mikhaleva, M. A.; Igonina, G. A.; Lazareva, V. T.; Rumyantsev, V. G.; Mamaev, V. P.
CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, 630090, Russia
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1993), (2), 209-14
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian

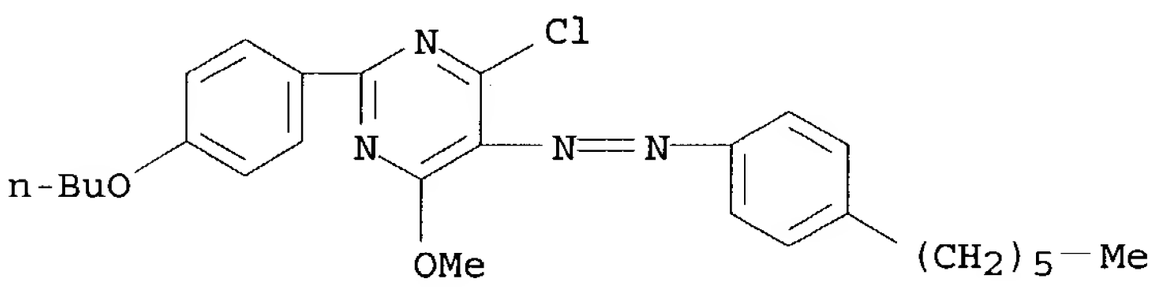
AB Substituted 5- and 2-(arylazo)pyrimidines were synthesized and studied for

potential application as dichroic dyes with pos. dichroism for color liquid-crystal. optical imaging devices. Absorption spectra (λmax = 368-474 nm) and order parameters (S = 0.38-0.71) were determined for 8 dyes. A dye with optimum properties (S = 0.71, λmax = 474 nm) is prepared by 2-[4-(hexyloxy)phenyl]-5-aminopyrimidine condensation with 1-(dimethylamino)-4-nitrosobenzene in superbasic medium.

IT **150563-33-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and characterization of, as potential dichroic dye for color liquid-crystal. optical imaging devices)

RN 150563-33-0 CAPLUS

CN Pyrimidine, 2-(4-butoxyphenyl)-4-chloro-5-[(4-hexylphenyl)azo]-6-methoxy- (9CI) (CA INDEX NAME)

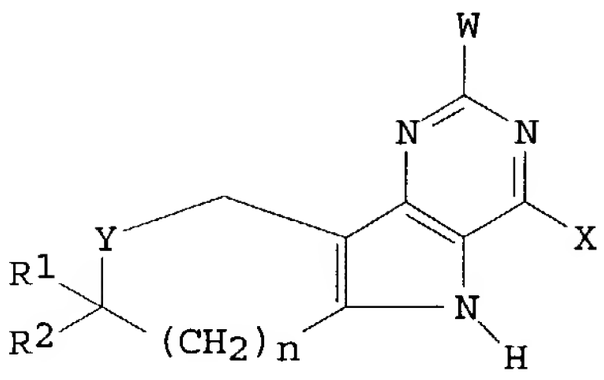



L10 ANSWER 25 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:448538 CAPLUS
DOCUMENT NUMBER: 117:48538
TITLE: Preparation of 6,7,8,9-tetrahydro-5H-indolo[3.2-d]pyrimidines and analogs as GABA receptor ligands
INVENTOR(S): Thurkauf, Andrew; Hutchison, Alan; Singh, Vinod
PATENT ASSIGNEE(S): Neurogen Corp., USA
SOURCE: PCT Int. Appl., 75 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9206094 | A1 | 19920416 | WO 1991-US7195 | 19911008 |
| W: AU, CA, JP, KR, US | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE | | | | |
| CA 2091986 | AA | 19920410 | CA 1991-2091986 | 19911008 |
| CA 2091986 | C | 19951128 | | |
| AU 9187326 | A1 | 19920428 | AU 1991-87326 | 19911008 |
| AU 652968 | B2 | 19940915 | | |
| EP 552237 | A1 | 19930728 | EP 1991-918267 | 19911008 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| JP 06502147 | T2 | 19940310 | JP 1991-517025 | 19911008 |
| EP 738717 | A1 | 19961023 | EP 1996-105337 | 19911008 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| US 5216159 | A | 19930601 | US 1991-800885 | 19911127 |
| CZ 281084 | B6 | 19960612 | CZ 1992-779 | 19920316 |
| CN 1076929 | A | 19931006 | CN 1992-102339 | 19920331 |
| IN 175034 | A | 19950422 | IN 1992-CA218 | 19920401 |
| US 5585490 | A | 19961217 | US 1993-30468 | 19930405 |

PRIORITY APPLN. INFO.: US 1990-594712 A2 19901009
EP 1991-918267 A3 19911008
WO 1991-US7195 A 19911008

OTHER SOURCE(S): MARPAT 117:48538
GI



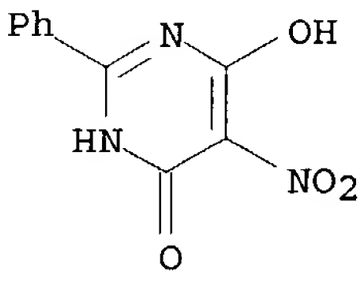
I

AB Title compds. I [n = 0-2; R1,R2 = H, C1-6 alkyl; X = H, OH; W = (substituted) Ph, -thienyl, -pyridyl; Y = NR3, CO, CR6OR5, CR6COR5, CR6CO2R5, CR6OCOR5R6, etc.; R3 = H, C1-6 alkyl, Ph, pyridyl, phenyl-C1-6 alkyl, aminoalkyl, 1-indanyl, etc.; R5 = H, C1-6 alkyl, Ph, pyridyl, phenyl-C1-6 alkyl; R6 = H, C1-6 alkyl] and related compds. were prepared as GABA receptor ligands. Thus, the enamine formed from cyclohexanone and pyrrolidine was arylated by treatment with 2-phenyl-5-nitro-4,6-dichloropyrimidine (preparation given) and (Me2CH)2EtN in CH2Cl2 and the product formed was hydrogenated in EtOH containing Et3N and 10% Pd/C to give 2-phenyl-6,7,8,9-tetrahydro-5H-indolo[3,2-d]-pyrimidine (II). II had IC50 of 0.100 μM against 3H-flumazenil binding to GABA receptors.

IT **68905-99-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for GABA receptor ligands)

RN 68905-99-7 CAPLUS

CN 4(1H)-Pyrimidinone, 6-hydroxy-5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 26 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:164270 CAPLUS
DOCUMENT NUMBER: 114:164270
TITLE: Preparation of phenylpyrimidone derivatives as inhibitors of a calmodulin-insensitive cyclic GMP phosphodiesterase
INVENTOR(S): Coates, William John
PATENT ASSIGNEE(S): Smith Kline and French Laboratories Ltd., UK
SOURCE: Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 400799 | A1 | 19901205 | EP 1990-304313 | 19900423 |
| EP 400799 | B1 | 19940112 | | |
| R: CH, DE, FR, GB, IT, LI, NL | | | | |
| JP 02295977 | A2 | 19901206 | JP 1990-109945 | 19900424 |
| US 5290933 | A | 19940301 | US 1991-794311 | 19911114 |

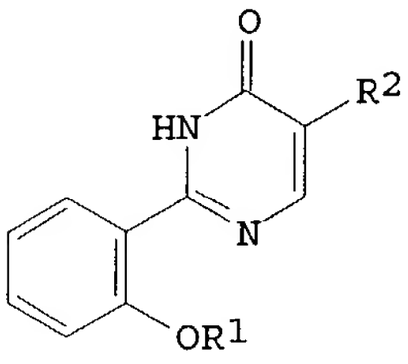
PRIORITY APPLN. INFO.: GB 1989-9558 19890426

09/ 811,359

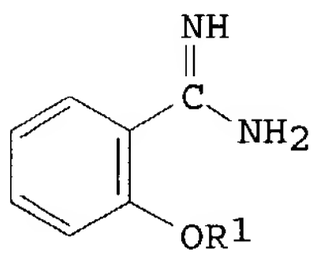
US 1990-514385 19900425

OTHER SOURCE(S): MARPAT 114:164270

GI



I



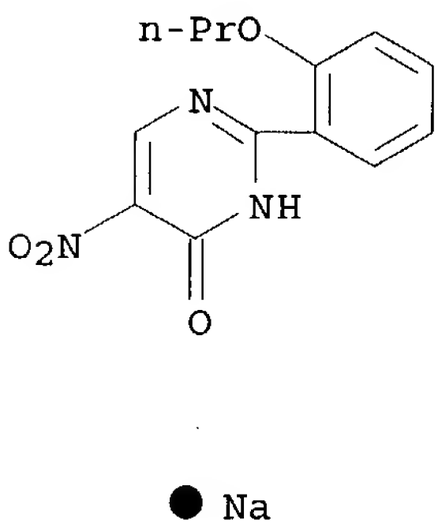
II

AB The title compds. (I; R1 = alkyl, alkenyl, cycloalkylalkyl, phenylalkyl, fluoroalkyl; R2 = H, NH2, alkanoylamino, CONR3R4; R4 = alkyl; R5 = H, alkyl), useful as vasodilators and antihypertensives and for treatment of asthma, bronchitis, and congestive heart failure, are prepared by cyclocondensation of benzamidines (II) with XCH:CR6CO2R7 (X = leaving group; R6 = any group R2 or its precursor; R7 = an ester forming group). Thus, cyclocondensation of II (R1 = Pr) with EtOCH:C(NO2)CO2Et in EtOH containing EtONa followed by acidification with aqueous HCl gave I (R2 = NO2) which was hydrogenated over 10 % Pd/C in MeOH to give I (R2 = NH2). I (R2 = AcNH) (II) at 3.8 μmol/kg reduced the U46619-induced bronchoconstriction by 50% in guinea-pigs. Soft gelatin capsules containing II were formulated.

IT **133152-11-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and acidification of)

RN 133152-11-1 CAPLUS

CN 4(1H)-Pyrimidinone, 5-nitro-2-(2-propoxyphenyl)-, sodium salt (9CI) (CA INDEX NAME)



● Na

L10 ANSWER 27 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:499389 CAPLUS

DOCUMENT NUMBER: 113:99389

TITLE: Metal-complex azo dyes for textile, leather and metal applications

INVENTOR(S): Puentener, Alois; Burdeska, Kurt

PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.

SOURCE: Eur. Pat. Appl., 21 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

09/ 811,359

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 357554 | A2 | 19900307 | EP 1989-810623 | 19890822 |
| EP 357554 | A3 | 19900912 | | |
| R: BE, CH, DE, ES, FR, GB, LI | | | | |
| US 4962191 | A | 19901009 | US 1989-399202 | 19890828 |
| JP 02117962 | A2 | 19900502 | JP 1989-226384 | 19890831 |

PRIORITY APPLN. INFO.: CH 1988-3238 19880831
OTHER SOURCE(S): MARPAT 113:99389
GI

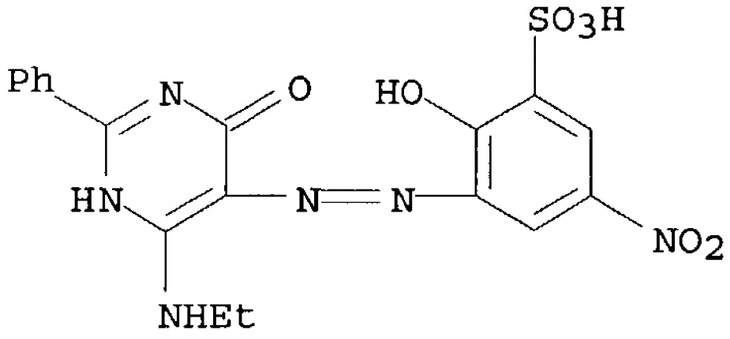
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title dyes I [D1, D2 = (un)substituted diazobenzene or naphthalene component having a OH or CO2H group ortho to the azo group; D3 = (un)substituted coupling benzene, naphthalene, or heterocyclic residue in which X is ortho to the azo group; M = Cr, Co; Q = (un)substituted Ph, naphthyl, or aromatic heterocyclic residue; R1 = (un)substituted C1-6 alkyl or Ph; R2 = H, R1; X = O, NR3; R3 = H, C1-4 alkyl; p, q = 0, 1], useful for dyeing rayon, natural cellulose fibers, protein fibers, polyimide fibers, polyurethane fibers, basic-modified polyolefin fibers, leather, pelts, or anodized Al, are prepared Thus, 3-amino-4-hydroxy-5-nitrobenzenesulfonic acid was diazotized and coupled with 4-(ethylamino)-6-hydroxy-2-phenylpyrimidine, and the azo intermediate complexed with Co sulfate, producing the 1:2 chrome-complex dye II, which dyed leather a fast red shade.

IT **129010-15-7P**
RL: PREP (Preparation)
(manufacture of, as intermediate for metal complex azo dyes)

RN 129010-15-7 CAPLUS

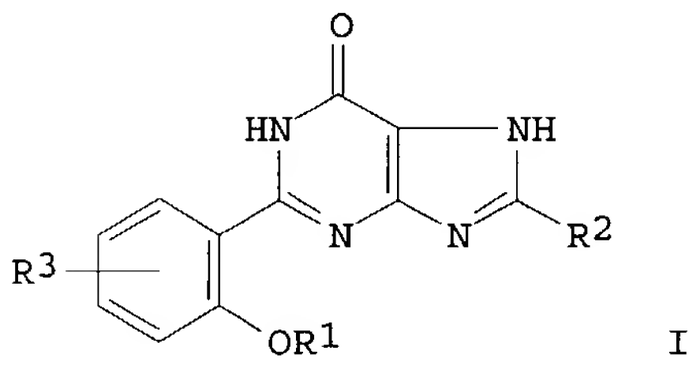
CN Benzenesulfonic acid, 3-[[6-(ethylamino)-1,4-dihydro-4-oxo-2-phenyl-5-pyrimidinyl]azo]-2-hydroxy-5-nitro- (9CI) (CA INDEX NAME)




L10 ANSWER 28 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:440713 CAPLUS
DOCUMENT NUMBER: 113:40713
TITLE: Alkoxyphenylpurines as inhibitors of calmodulin-insensitive cyclic GMP phosphodiesterase
INVENTOR(S): Coates, William John
PATENT ASSIGNEE(S): Smith Kline and French Laboratories Ltd., UK
SOURCE: Eur. Pat. Appl., 17 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 352960 | A2 | 19900131 | EP 1989-307341 | 19890719 |
| EP 352960 | A3 | 19911106 | | |
| EP 352960 | B1 | 19941026 | | |
| R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| AU 8938210 | A1 | 19900125 | AU 1989-38210 | 19890718 |
| AU 613503 | B2 | 19910801 | | |
| US 5073559 | A | 19911217 | US 1989-382610 | 19890719 |
| DK 8903636 | A | 19900126 | DK 1989-3636 | 19890721 |
| ZA 8905613 | A | 19900530 | ZA 1989-5613 | 19890724 |
| JP 02088577 | A2 | 19900328 | JP 1989-192462 | 19890725 |

PRIORITY APPLN. INFO.: GB 1988-17651 19880725
OTHER SOURCE(S): MARPAT 113:40713
GI

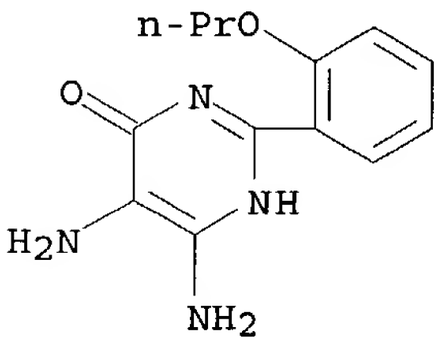


I

AB The title compds. [I; R1 = (fluoro)alkyl, alkenyl, cycloalkylalkyl, phenylalkyl; R2 = H, OH, alkyl, Ph, SH, alkylthio, CF3, amino; R3 = H, NO2, amino, alkanoylamino, alkoxy, alkyl, halo, SO2NR4R5, CONR4R5, alkylthio, alkylsulfonyl, CN, etc.; R4, R5 = H, alkyl] were prepared as inhibitors of calmodulin-insensitive cyclic GMP phosphodiesterase. Thus, 2-(2-propxy-5-chlorophenyl)purin-6-one (II) was prepared in 6 steps from 5-chloro-2-hydroxybenzamide via 2-(5-chloro-2-propxyphenyl)-4-amino-5-nitrosopyrimidin-6-one. II at 16.6 μmol/kg i.v. in guinea pigs gave 30% inhibition of ovalbumin-induced bronchoconstriction. A capsule formulation containing II is given.

IT **57075-34-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with acetamidine hydrochloride)

RN 57075-34-0 CAPLUS
CN 4(1H)-Pyrimidinone, 5,6-diamino-2-(2-propoxyphenyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 29 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:423942 CAPLUS
DOCUMENT NUMBER: 113:23942
TITLE: Preparation of condensed pyrimidine derivatives as inhibitors of calmodulin insensitive cyclic GMP

phosphodiesterase

INVENTOR(S): Coates, William John; Rawlings, Derek Anthony
PATENT ASSIGNEE(S): Smith Kline and French Laboratories Ltd., UK
SOURCE: Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 349239 | A2 | 19900103 | EP 1989-306453 | 19890626 |
| EP 349239 | A3 | 19900718 | | |
| EP 349239 | B1 | 19940316 | | |
| R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| US 5075310 | A | 19911224 | US 1989-370494 | 19890623 |
| AT 102945 | E | 19940415 | AT 1989-306453 | 19890626 |
| AU 8937099 | A1 | 19900104 | AU 1989-37099 | 19890627 |
| AU 614389 | B2 | 19910829 | | |
| DK 8903228 | A | 19900102 | DK 1989-3228 | 19890628 |
| ZA 8904942 | A | 19910626 | ZA 1989-4942 | 19890629 |
| JP 02056484 | A2 | 19900226 | JP 1989-171017 | 19890630 |

PRIORITY APPLN. INFO.: GB 1988-15716 19880701
GB 1988-15717 19880701
GB 1988-15718 19880701
EP 1989-306453 19890626

OTHER SOURCE(S): MARPAT 113:23942
GI For diagram(s), see printed CA Issue.

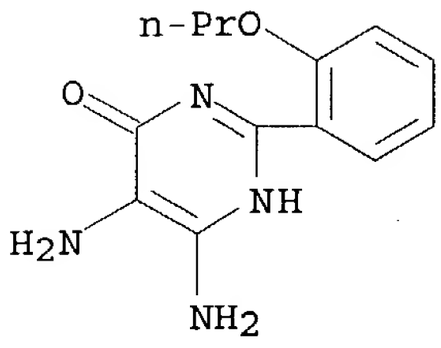
AB The title compds. (I; ring A = Q-Q2; X = O, S; R1 = C1-6 alkyl, C2-6 alkenyl, C3-5 cycloalkyl, C1-4 alkyl, C1-4 alkyl substituted by 1-6 F), useful for treatment of asthma and bronchitis and also as vasodilators in treatment of angina, hypertension, and congestive heart failure, are prepared by (1) cyclocondensation of 2-R1OC6H4R2 [II; R2 = C(:NH)NH2] with a pyrazole derivative (III; R3 = C1-4 alkoxy, NH2) to give I (ring A = Q), (2) cyclization of II (R2 = Q3) to give I (ring A = Q, Q1), (3) oxidative cyclization of II (R2 = Q4, X1 = nitroso) to give I (ring A = Q2, X = O), and (4) cyclocondensation of II (R2 = Q4, X1 = NH2) with SOCl2 to give I (ring A = Q2, X = S). Thus, a mixture of II [R1 = Pr, R2 = C(:NH)NH2].MeSO3H, II (R3 = NH2).H2SO4, and AcONa was heated 1 h in an oil bath (180°) to give I (R1 = Pr, ring A = Q). Also prepared were I (R1 = Pr; ring A = Q1, Q2 where X = O, S). Three I at 2.62-5.13 μmol/kg inhibited 50% the bronchoconstriction induced by U46619 (9,11-methanoepoxy-PGH2) in guinea pigs.

IT **119409-17-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with thionyl chloride)

RN 119409-17-5 CAPLUS
CN 4(1H)-Pyrimidinone, 5,6-diamino-2-(2-propoxyphenyl)-, sulfate (9CI) (CA INDEX NAME)

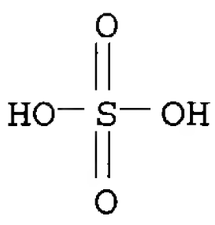
CM 1

CRN 57075-34-0
CMF C13 H16 N4 O2




CM 2

CRN 7664-93-9
CMF H2 O4 S




L10 ANSWER 30 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:406363 CAPLUS
DOCUMENT NUMBER: 113:6363
TITLE: Fused pyrimidine derivatives, process and intermediates for their preparation and pharmaceutical compositions containing them
INVENTOR(S): Coates, William John; Flynn, Seyn Thomas; Rawlings, Derek Anthony
PATENT ASSIGNEE(S): Smith Kline and French Laboratories Ltd., UK
SOURCE: Eur. Pat. Appl., 29 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 347146 | A2 | 19891220 | EP 1989-305911 | 19890612 |
| EP 347146 | A3 | 19900711 | | |
| EP 347146 | B1 | 19930901 | | |
| R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| AT 93858 | E | 19930915 | AT 1989-305911 | 19890612 |
| ES 2058527 | T3 | 19941101 | ES 1989-305911 | 19890612 |
| US 5047404 | A | 19910910 | US 1989-365469 | 19890613 |
| AU 8936357 | A1 | 19891221 | AU 1989-36357 | 19890614 |
| AU 612852 | B2 | 19910718 | | |
| DK 8902970 | A | 19891217 | DK 1989-2970 | 19890615 |
| ZA 8904563 | A | 19910130 | ZA 1989-4563 | 19890615 |
| JP 02042079 | A2 | 19900213 | JP 1989-155560 | 19890616 |
| JP 2815617 | B2 | 19981027 | | |

PRIORITY APPLN. INFO.: GB 1988-14350 A 19880616
GB 1988-14351 A 19880616
GB 1988-14353 A 19880616
EP 1989-305911 A 19890612
OTHER SOURCE(S): MARPAT 113:6363
GI For diagram(s), see printed CA Issue.

09/ 811,359

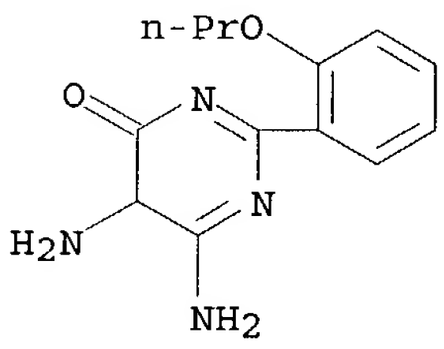
AB Title compds. I [R1 = (substituted C1-6 alkyl, C2-6 alkenyl, C3-5 cycloalkyl-C1-6 alkyl; R2 = C1-6 alkylthio, C1-6 alkylsulfonyl, C1-6 alkoxy, HO, H, H2NNH, C1-6 alkyl, Ph, R3CONH, R3 = H, C1-6 alkyl, R4R5N = pyrrolidino, piperidino, morpholino, etc.; A = pyrido, (substituted) pyrazino, triazino] are prepared as bronchodilators, antiallergics, vasodilators, and inhibitors of a calmodulin insensitive cyclic GMP phosphodiesterase. 2-PrOC6H4COCl in MeCN was added dropwise to 2-aminonicotinamide and Et3N in MeCN to give 2-(2-propoxybenzamido)nicotinamide which with pyridine in 2N NaOH was refluxed for 30 min to give II, which was effective in controlling allergic reactions at 28 μmol/kg i.v. in guinea pigs. Also prepared were 22 addnl. I which showed bronchodilation, vasodilation, antiallergy activity and phosphodiesterase inhibition. A capsule formulation comprising II was given.

IT **127488-22-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of fused pyrimidine pharmaceuticals)

RN 127488-22-6 CAPLUS
CN 4(5H)-Pyrimidinone, 5,6-diamino-2-(2-propoxyphenyl)-, sulfate (1:1) (9CI) (CA INDEX NAME)

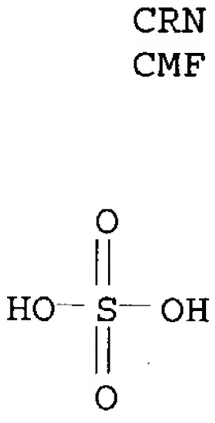
CM 1

CRN 127488-21-5
CMF C13 H16 N4 O2




CM 2

CRN 7664-93-9
CMF H2 O4 S




L10 ANSWER 31 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:114815 CAPLUS
DOCUMENT NUMBER: 110:114815
TITLE: Preparation and formulation of 2-(2-alkoxyphenyl)-6-purinone derivatives as pharmaceuticals
PATENT ASSIGNEE(S): Smith Kline and French Laboratories Ltd., UK
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

09/ 811,359

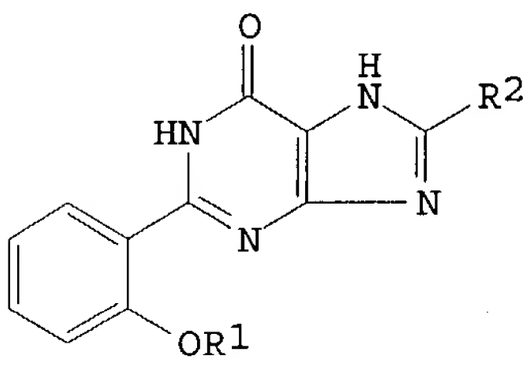
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 63196585 | A2 | 19880815 | JP 1988-23631 | 19880201 |
| CA 1303037 | A1 | 19920609 | CA 1988-557327 | 19880126 |
| DK 8800407 | A | 19880803 | DK 1988-407 | 19880127 |
| EP 293063 | A1 | 19881130 | EP 1988-300696 | 19880127 |
| EP 293063 | B1 | 19920318 | | |
| R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| US 4885301 | A | 19891205 | US 1988-148791 | 19880127 |
| AT 73802 | E | 19920415 | AT 1988-300696 | 19880127 |
| ES 2033423 | T3 | 19930316 | ES 1988-300696 | 19880127 |
| AU 8810956 | A1 | 19880804 | AU 1988-10956 | 19880129 |
| AU 599452 | B2 | 19900719 | | |
| ZA 8800680 | A | 19880928 | ZA 1988-680 | 19880201 |

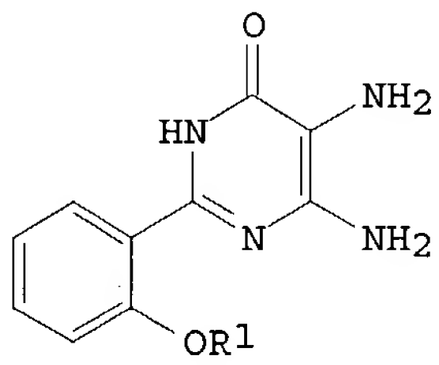
PRIORITY APPLN. INFO.: GB 1987-2300 19870202
GB 1987-2301 19870202
EP 1988-300696 19880127

OTHER SOURCE(S): MARPAT 110:114815

GI




I



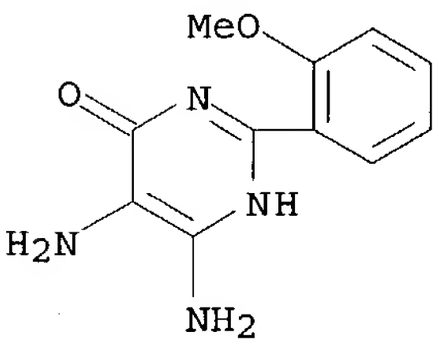

II

AB The title compds. (I; R1 = C1-6 alkyl, C2-6 alkenyl; R2 = H, OH), useful as bronchodilators and vasodilators, are prepared A mixture of 1.5 g diaminopyrimidinone salt II.H2SO4 (R1 = Pr) and HCONH2 was heated 70 min at 190-200° to give 0.72 g purinone I (R1 = Pr, R2 = H) (III), which had an ED50 of 3.6 μmol/kg against bronchoconstriction in guinea pigs and an IC50 of 0.96 μM for inhibition of phosphodiesterase extracted from pig arteries. Soft gelatin capsules were prepared each containing III 3.0, soy bean oil 88.2, and hydrogenated vegetable shortening-beeswax 8.8 weight%.

IT **57075-32-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with amides)

RN 57075-32-8 CAPLUS

CN 4(1H)-Pyrimidinone, 5,6-diamino-2-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



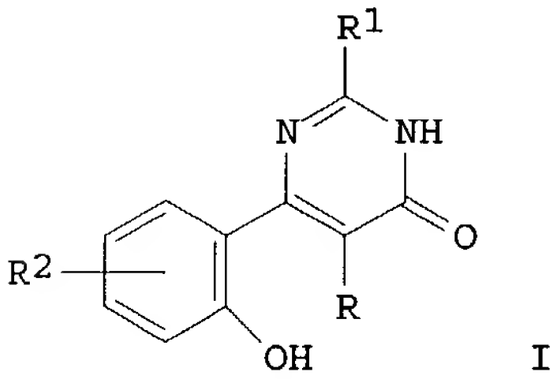

L10 ANSWER 32 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:611073 CAPLUS

09/ 811,359

DOCUMENT NUMBER: 109:211073
TITLE: Preparation and testing of 5-amino-6-(2-hydroxyphenyl)pyrimidin-4(3H)-one derivatives as analgesics
INVENTOR(S): Tanaka, Masaaki; Ogura, Kuniyoshi; Morita, Hikari; Aozuka, Tomoshi; Nakada, Naoki; Takagi, Kaname
PATENT ASSIGNEE(S): Zeria Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 63030473 | A2 | 19880209 | JP 1986-173555 | 19860725 |

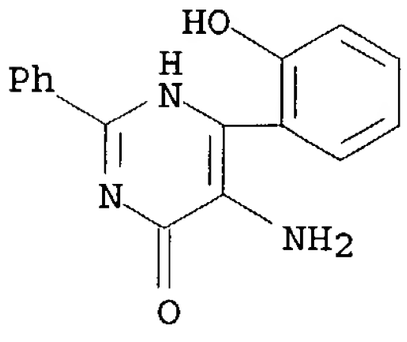
PRIORITY APPLN. INFO.: JP 1986-173555 19860725
OTHER SOURCE(S): MARPAT 109:211073
GI




I

AB The title compds. [I; R = NH2, R1 = lower alkyl, (un)substituted Ph, NH2, cyclic amino; R2 = H, lower alkyl, lower alkoxy, halo] (II) were prepared as analgesics. MeC(:NH)NH2·HCl was added to a solution of Na in EtOH and the mixture was stirred at room temperature for 10 min. To the mixture, 4-methoxy-3-nitrocoumarin was added and the mixture was refluxed for 1 h to give 70% I (R = NO2, R1 = Me, R2 = H) which was hydrogenated over 5% Pd/C in EtOH to give 50% I (R = NH2, R1 = Me, R2 = H) (IV). IV at 30 mg/kg p.o. exhibited 68.3% inhibition of AcOH-induced writhing in mice whereas aminopyrine showed 38.9% inhibition.

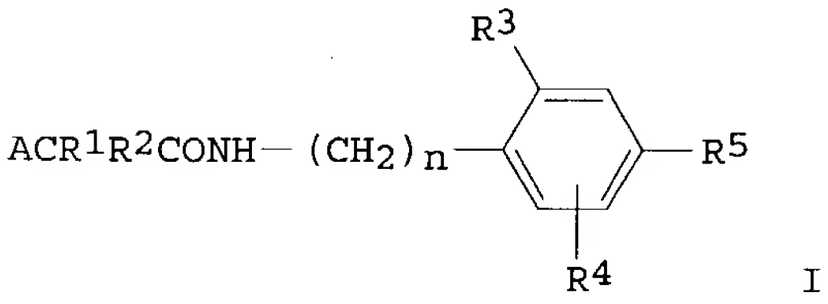
IT **110566-03-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as analgesic)
RN 110566-03-5 CAPLUS
CN 4(1H)-Pyrimidinone, 5-amino-6-(2-hydroxyphenyl)-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 33 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:417030 CAPLUS
DOCUMENT NUMBER: 109:17030
TITLE: Saturated fatty acid amides as inhibitors of acyl-CoA:cholesterol acyltransferase
INVENTOR(S): Hoefle, Milton L.; Holmes, Ann; Roth, Bruce D.
PATENT ASSIGNEE(S): Warner-Lambert Co., USA
SOURCE: U.S.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 4716175 | A | 19871229 | US 1987-17960 | 19870224 |
| US 4743605 | A | 19880510 | US 1987-103316 | 19871001 |
| CA 1336913 | A1 | 19950905 | CA 1988-557467 | 19880127 |
| ZA 8800604 | A | 19890927 | ZA 1988-604 | 19880128 |
| AU 8811354 | A1 | 19880825 | AU 1988-11354 | 19880205 |
| AU 610558 | B2 | 19910523 | | |
| FI 8800796 | A | 19880825 | FI 1988-796 | 19880219 |
| FI 89593 | B | 19930715 | | |
| FI 89593 | C | 19931025 | | |
| DK 8800941 | A | 19880825 | DK 1988-941 | 19880223 |
| DK 165406 | B | 19921123 | | |
| DK 165406 | C | 19930413 | | |
| NO 8800774 | A | 19880825 | NO 1988-774 | 19880223 |
| NO 174043 | B | 19931129 | | |
| NO 174043 | C | 19940309 | | |
| EP 283742 | A2 | 19880928 | EP 1988-102644 | 19880223 |
| EP 283742 | A3 | 19890726 | | |
| EP 283742 | B1 | 19930526 | | |
| R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| JP 63253060 | A2 | 19881020 | JP 1988-38777 | 19880223 |
| JP 07121895 | B4 | 19951225 | | |
| AT 89814 | E | 19930615 | AT 1988-102644 | 19880223 |
| ES 2056843 | T3 | 19941016 | ES 1988-102644 | 19880223 |
| US 4716175 | B1 | 19930622 | US 1990-90002032 | 19900529 |

PRIORITY APPLN. INFO.: US 1987-17960 19870224
EP 1988-102644 19880223
OTHER SOURCE(S): CASREACT 109:17030
GI

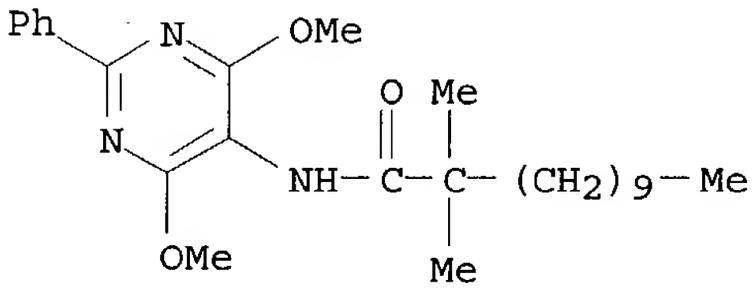


I

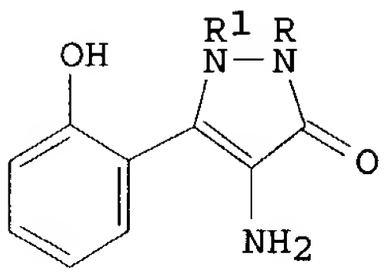
II

AB Title phenylalkyl amides I and pyridylalkyl amides II (A = C1-20 hydrocarbyl containing 1-3 double bonds; R1 = H, C1-4 alkyl, PhCH2; R2 = C1-4 alkyl, PhCH2; CR1R2 = saturated C3-7 carbocyclic ring; R3-R5 = H, F, Cl, Br, CF3, C1-4 alkyl, C1-4 alkoxy, n = 0, 1) are prepared, and are useful for inhibiting intestinal absorption of cholesterol. MeCH(CO2Et)2 was treated with NaOEt, and alkylated with 1-bromotetradecane, followed by hydrolysis to give 2-methyl-2-tetradecylmalonic acid, which was thermally decarboxylated to form 2-methylhexadecanoic acid. The latter compound was transformed into the acid chloride and treated with 2,4,6-trimethoxyphenylamine-HCl to form N-(2,4,6-trimethoxyphenyl)-2-methylhexadecanamide. 2,2-Dimethyl-N-(2,4,6-trimethoxyphenyl)dodecanamide (50 mg/kg) was administered orally 30 min prior to each meal to cholesterol-loaded rabbits fed a high cholesterol diet; after 7 days, there was a 67% decrease in serum cholesterol, compared to cholesterol-loaded nontreated controls.

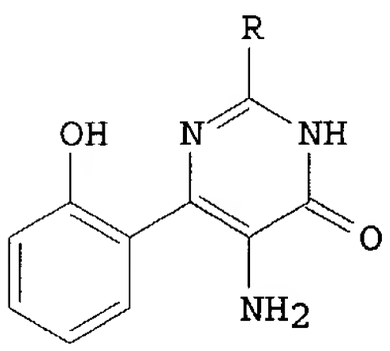
IT **114289-67-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for inhibition of absorption of dietary cholesterol)
RN 114289-67-7 CAPLUS
CN Dodecanamide, N-(4,6-dimethoxy-2-phenyl-5-pyrimidinyl)-2,2-dimethyl- (9CI) (CA INDEX NAME)




L10 ANSWER 34 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1987:547168 CAPLUS
DOCUMENT NUMBER: 107:147168
TITLE: Synthesis and analgesic activity of 4-amino-1,2-dihydro-5-(2-hydroxyphenyl)-3H-pyrazol-3-ones and 5-amino-6-(2-hydroxyphenyl)pyrimidin-4(3H)-ones
AUTHOR(S): Takagi, Kaname; Tanaka, Masaaki; Morita, Hikari; Ogura, Kuniyoshi; Ishii, Katsuyuki; Nakata, Naoki; Ozeki, Masayuki
CORPORATE SOURCE: Cent. Res. Lab., Zeria Pharm. Co., Saitama, 360-01, Japan
SOURCE: European Journal of Medicinal Chemistry (1987), 22(3), 239-42
CODEN: EJMCA5; ISSN: 0223-5234
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:147168
GI



I, R=R1=H
II, R=Me, R1=H
III, R=H, R1=Me



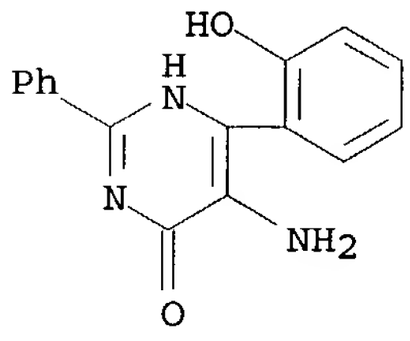
IV, R=Me
V, R=C6H4NH2-4

AB Three 4-amino-1,2-dihydro-5-(2-hydroxyphenyl)-3-H-pyrazol-3-ones and six 5-amino-6-(2-hydroxyphenyl)pyrimidin-4(3H)-ones were synthesized from 4-methoxy- and 4-hydroxy-3-nitrocoumarins, and tested for analgesic activity upon oral administration to mice. Most of the compds. prepared exhibited analgesic activity which was superior to that of aminopyrine. In particular, the pyrazolones I, II, and III and the pyrimidinones IV and V, showed prominent activity, which was 3-4.5 times as potent as that of aminopyrine.

IT **110566-03-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and analgesic activity of)

RN 110566-03-5 CAPLUS

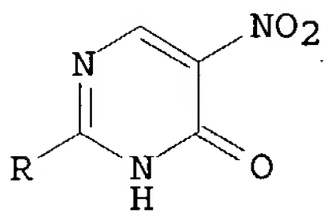
CN 4(1H)-Pyrimidinone, 5-amino-6-(2-hydroxyphenyl)-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 35 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:129853 CAPLUS
DOCUMENT NUMBER: 104:129853
TITLE: Synthesis of 2-substituted 4-oxo-5-nitropyrimidines from methyl 3-ethoxy-2-nitroacrylate and other reactions
AUTHOR(S): De la Cuesta, E.; Avendano, C.
CORPORATE SOURCE: Fac. Farm., Univ. Complutense, Madrid, Spain
SOURCE: Journal of Heterocyclic Chemistry (1985), 22(2), 337-9
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:129853

GI



I

AB Nitropyrimidines I (R = NH2, Me, Ph) were prepared by cyclization of EtOCH:C(NO2)CO2Me (II) and HN:CR(NH2). Condensation of II with H2NNHCOR1 (R1 = Me, Ph) yielded R1CONHNHCH:C(NO2)CO2Me which could not be cyclized.

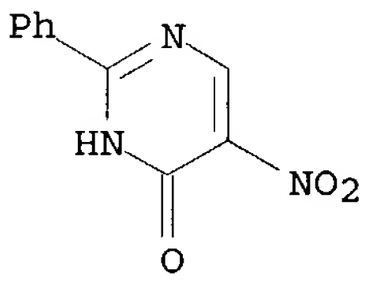
IT **99893-00-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and neutralization of, with acetic acid)

RN 99893-00-2 CAPLUS

CN Benzenecarboximidamide, compd. with 5-nitro-2-phenyl-4(1H)-pyrimidinone (1:1) (9CI) (CA INDEX NAME)

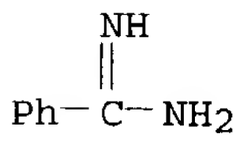
CM 1

CRN 3749-46-0
CMF C10 H7 N3 O3



CM 2

CRN 618-39-3
CMF C7 H8 N2



L10 ANSWER 36 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1985:406360 CAPLUS
DOCUMENT NUMBER: 103:6360
TITLE: N-(2-Nitrophenyl)-5-aminopyrimidine derivatives and their use
INVENTOR(S): Zondler, Helmut; Hubele, Adolf; Nyfeler, Robert
PATENT ASSIGNEE(S): Ciba-Geigy A.-G. , Switz.
SOURCE: Eur. Pat. Appl., 92 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1

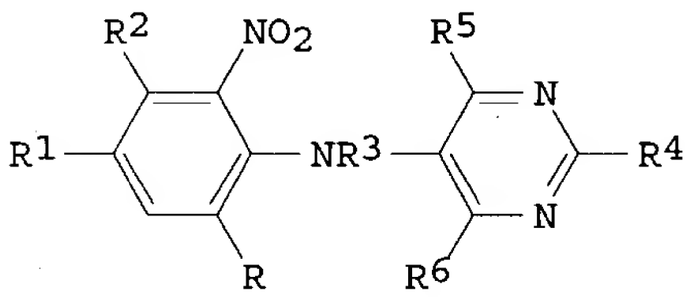
09/ 811,359

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 132826 | A1 | 19850213 | EP 1984-108700 | 19840723 |
| EP 132826 | B1 | 19880928 | | |
| R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE | | | | |
| US 4840662 | A | 19890620 | US 1984-631272 | 19840716 |
| IL 72478 | A1 | 19871220 | IL 1984-72478 | 19840720 |
| CA 1218370 | A1 | 19870224 | CA 1984-459440 | 19840723 |
| AT 37540 | E | 19881015 | AT 1984-108700 | 19840723 |
| DK 8403620 | A | 19850126 | DK 1984-3620 | 19840724 |
| AU 8430998 | A1 | 19850214 | AU 1984-30998 | 19840724 |
| AU 577053 | B2 | 19880915 | | |
| ZA 8405703 | A | 19850327 | ZA 1984-5703 | 19840724 |
| BR 8403677 | A | 19850702 | BR 1984-3677 | 19840724 |
| ES 534577 | A1 | 19850716 | ES 1984-534577 | 19840724 |
| JP 60051178 | A2 | 19850322 | JP 1984-155129 | 19840725 |

PRIORITY APPLN. INFO.: CH 1983-4047 19830725
EP 1984-108700 19840723

GI



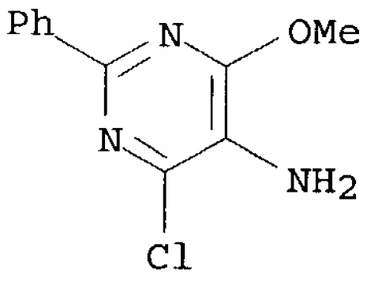

I

AB Seventy-four title compds. I [R, R1 = H, NO2, CF3; R2 = H, halo; R3 = H, COR7 [R7 = (un)substituted alkyl]; R4 = H, halo, NO2, cyano, SH, thiocyanato, alkyl, haloalkyl, substituted cycloalkoxy, alkenyloxy, alkynyloxy, alkylthio, alkenylthio, alkylsulfonyl, alkylsulfinyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl, dialkylamino, (un)substituted alkoxy, Ph, PhCH2; R5, R6 = H, halo, NO2, cyano, SH, thiocyanato, alkyl, haloalkyl, (un)substituted alkoxy, substituted cycloalkoxy, alkenyloxy, alkynyloxy, alkylthio, alkenylthio, alkylsulfonyl, alkylsulfinyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl, dialkylamino] were prepared Thus, 2.84 g 5-amino-4-chloro-6-methoxypyrimidine in 20 mL DMSO at 15° was treated dropwise with 6.24 g 1,3-dichloro-2,6-dinitro-4-(trifluoromethyl)benzene and 2.30 g KOCMe3 in 15 mL DMSO to give 2.52 g I (R = NO2, R1 = CF3, R2 = R5 = Cl, R3 = R4 = H, R6 = OMe), which at 0.02% inhibited Puccinia graminis on wheat by 95-100%.

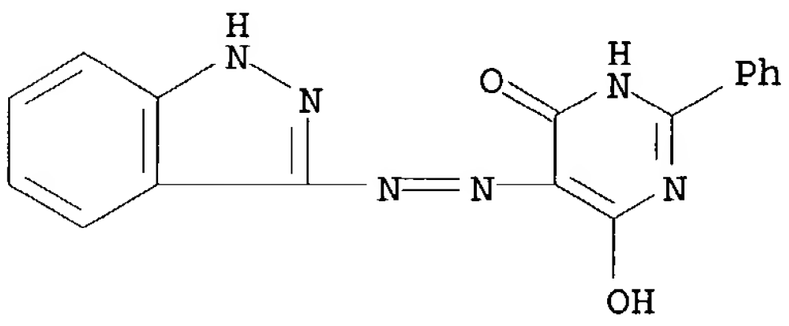
IT **96833-44-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination by, of chlorobenzene derivative)

RN 96833-44-2 CAPLUS

CN 5-Pyrimidinamine, 4-chloro-6-methoxy-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 37 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1985:150903 CAPLUS
DOCUMENT NUMBER: 102:150903
TITLE: Fluorescent dyes for solar collectors
AUTHOR(S): Iden, Ruediger; Seybold, Guenther; Stange, Andreas; Eilingsfeld, Heinz
CORPORATE SOURCE: ZD/Farbenlab., BASF A.-G., Ludwigshafen, Fed. Rep. Ger.
SOURCE: Forschungsber. - Bundesminist. Forsch. Technol., Technol. Forsch. Entwickl. (1984), BMFT-FB-T 84-164, 115 pp.
CODEN: BFTEAJ; ISSN: 0340-7608
DOCUMENT TYPE: Report
LANGUAGE: German
AB A large number of organic dyes was synthesized and screened for potential use in solar collectors. Most suitable were perylene and perylene imide dyes, B complexes of naphtholactam dyes, and polycarbocyclic dyes. These compds. covered the whole color range from yellow to blue. Chromatog. methods were developed for purification of fluorescent dyes.
IT **95689-94-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 95689-94-4 CAPLUS
CN 4(1H)-Pyrimidinone, 6-hydroxy-5-(1H-indazol-3-ylazo)-2-phenyl- (9CI) (CA INDEX NAME)

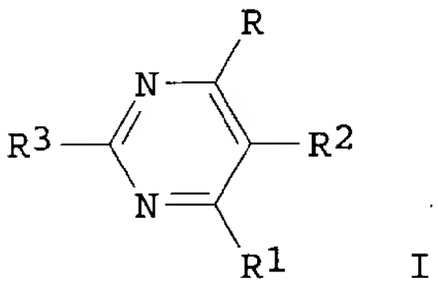



L10 ANSWER 38 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1984:591957 CAPLUS
DOCUMENT NUMBER: 101:191957
TITLE: 2-Aryl-4,6-dihalopyrimidines as antidotes for protecting cultivated plants from damage by herbicides
INVENTOR(S): Brunner, Hans Georg
PATENT ASSIGNEE(S): Ciba-Geigy A.-G. , Switz.
SOURCE: Eur. Pat. Appl., 42 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 112280 | A2 | 19840627 | EP 1983-810514 | 19831109 |
| EP 112280 | A3 | 19850925 | | |
| EP 112280 | B1 | 19900829 | | |
| R: BE, CH, DE, FR, GB, IT, LI, NL | | | | |
| US 4648896 | A | 19870310 | US 1983-549038 | 19831107 |
| CA 1233819 | A1 | 19880308 | CA 1983-440899 | 19831110 |
| BR 8306261 | A | 19840619 | BR 1983-6261 | 19831114 |
| ZA 8308467 | A | 19840627 | ZA 1983-8467 | 19831114 |

| | | | | |
|---|---|---|---|---|
| ES 527234 | A1 | 19851116 | ES 1983-527234 | 19831114 |
| IL 70231 | A1 | 19890630 | IL 1983-70231 | 19831114 |
| JP 59104365 | A2 | 19840616 | JP 1983-214945 | 19831115 |
| PRIORITY APPLN. INFO.: | | | CH 1982-6650 | 19821115 |
| | | | IL 1981-64612 | 19811221 |

GI



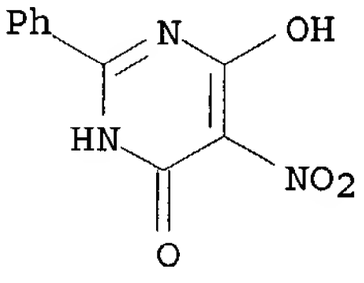
I

AB The title compds. [I; R, R1 = halo; R2 = amino, acyl, thiocyanato, R4Z (R4 = H, acyl, alkynyl, (un)substituted alkyl, alkenyl; Z = O, S, SO, SO2), R3 = (un)substituted Ph, thienyl, furyl] were prepared Thus, 2-phenyl-4,6-pyrimidinediol was nitrated to give I (R = R1 = OH, R2 = NO2, R3 = Ph). This was chlorinated by POCl3 in the presence of PhNMe2 and hydrogenated over Raney Ni to give I (R = R1 = Cl, R2 = NH2, R3 = Ph) (II). At 100 ppm II gave 50% protection to rice seedlings treated with the herbicide pretilachlor at 0.25 kg/ha.

IT **68905-99-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)

RN 68905-99-7 CAPLUS

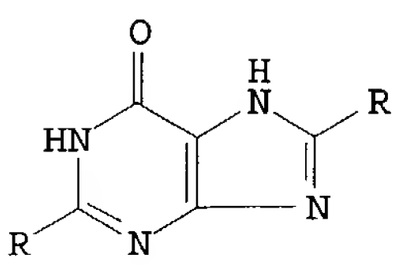
CN 4(1H)-Pyrimidinone, 6-hydroxy-5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



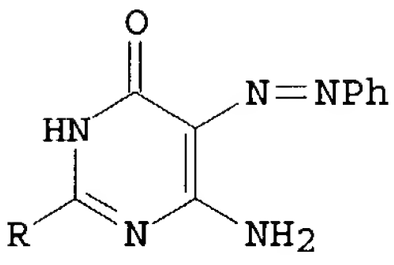
L10 ANSWER 39 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

| | |
|---|---|
| ACCESSION NUMBER: | 1982:406048 CAPLUS |
| DOCUMENT NUMBER: | 97:6048 |
| TITLE: | A one-step synthesis of purine derivatives by the reaction of phenylazomalonamidamidine with aryl aldehydes |
| AUTHOR(S): | Yoneda, Fumio; Koga, Ryosuke; Higuchi, Masatsugu |
| CORPORATE SOURCE: | Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, 862, Japan |
| SOURCE: | Chemistry Letters (1982), (3), 365-8<br>CODEN: CMLTAG; ISSN: 0366-7022 |
| DOCUMENT TYPE: | Journal |
| LANGUAGE: | English |
| OTHER SOURCE(S): | CASREACT 97:6048 |

GI



I



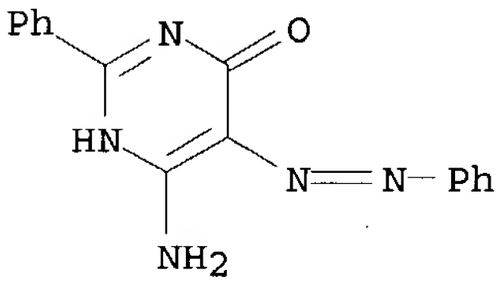
II

AB Treatment of H2NCOCH(N:NPh)C(:NH)NH2.HCl with RCHO (R = Ph, substituted Ph) yielded the 2,8-diarylhypoxanthines I in a single step. Under milder conditions the reaction formed H2NCOCH(N:NPh)C(:NH)N:CHR.HCl, from which the phenylazopyrimidine-4(3H)-ones II were obtained by oxidative cyclization with EtO2CN:NCO2Et. Treatment of II with a second aryl aldehyde gave the unsym. 2,8-diarylated hypoxanthines.

IT **54014-72-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with aromatic aldehydes)

RN 54014-72-1 CAPLUS

CN 4(1H)-Pyrimidinone, 6-amino-2-phenyl-5-(phenylazo)- (9CI) (CA INDEX NAME)



L10 ANSWER 40 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1980:639357 CAPLUS

DOCUMENT NUMBER: 93:239357

TITLE: Use of the Vilsmeier reaction in the synthesis of pyrrolo [3,2-d]pyrimidine-7-aldehyde derivatives

AUTHOR(S): Sizova, O. S.; Britikova, N. E.; Novitskii, K. Yu.; Shcherbakova, L. I.; Pershin, G. N.

CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR

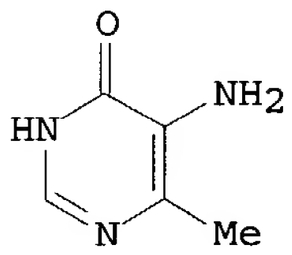
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1980), 14(7), 63-6
CODEN: KHFZAN; ISSN: 0023-1134

DOCUMENT TYPE: Journal

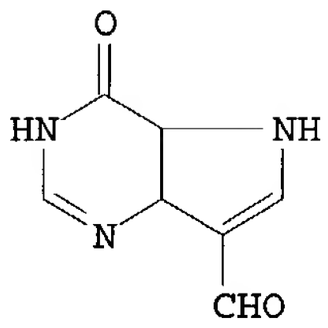
LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 93:239357

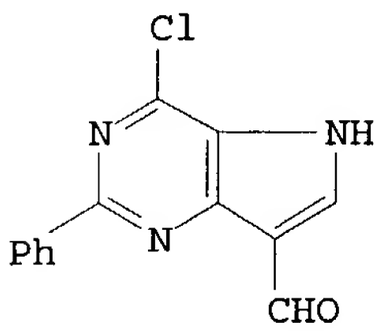
GI



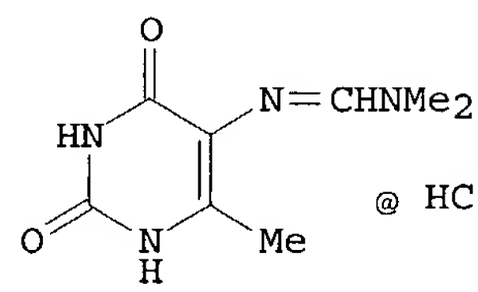
I



II



III



@ HCl

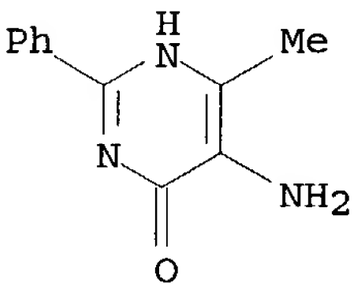
IV

AB Vilsmeier reaction of pyrimidinone I, prepare from thiourea and MeCOCH(NHAc)CO2Et via a pyrimidinethione, gave 70% aldehyde II. Aldehyde III was prepared similarly. Formamidine IV was prepared by Vilsmeier reaction of 5-amino-6-methyluracil. The phenylhydrazones of III suppressed the growth of lactic acid bacteria.

IT **72168-62-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(Vilsmeier reaction of)

RN 72168-62-8 CAPLUS

CN 4(1H)-Pyrimidinone, 5-amino-6-methyl-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 41 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1980:604635 CAPLUS

DOCUMENT NUMBER: 93:204635

TITLE: Penicillins and their salts

INVENTOR(S): Wetzel, Bernd; Woitun, Eberhard; Reuter, Wolfgang; Maier, Roland; Lechner, Uwe; Goeth, Hanns

PATENT ASSIGNEE(S): Thomae, Dr. Karl, G.m.b.H., Fed. Rep. Ger.

SOURCE: Ger. Offen., 53 pp. Addn. to Ger. Offen. 2,808,153.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 2851270 | A1 | 19800612 | DE 1978-2851270 | 19781127 |
| ES 477520 | A1 | 19790601 | ES 1979-477520 | 19790207 |
| EP 3814 | A2 | 19790905 | EP 1979-100468 | 19790219 |
| EP 3814 | A3 | 19791017 | | |
| EP 3814 | B1 | 19811216 | | |

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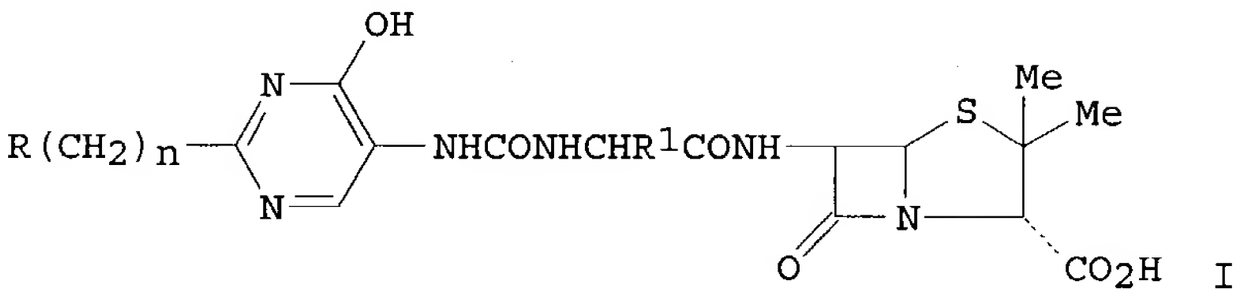
R: BE, CH, DE, FR, GB, IT, LU, NL, SE

| | | | | |
|---|---|---|---|---|
| AT 7901282 | A | 19810315 | AT 1979-1282 | 19790220 |
| AT 364459 | B | 19811027 | | |
| US 4241056 | A | 19801223 | US 1979-13006 | 19790221 |
| DK 7900774 | A | 19790826 | DK 1979-774 | 19790222 |
| FI 7900614 | A | 19790826 | FI 1979-614 | 19790223 |
| FI 68237 | B | 19850430 | | |
| FI 68237 | C | 19850812 | | |
| NO 7900628 | A | 19790828 | NO 1979-628 | 19790223 |
| AU 7944559 | A1 | 19790920 | AU 1979-44559 | 19790223 |
| AU 522042 | B2 | 19820513 | | |
| IL 56731 | A1 | 19820430 | IL 1979-56731 | 19790223 |
| HU 23633 | O | 19820928 | HU 1979-TO1096 | 19790223 |
| HU 180997 | B | 19830530 | | |
| JP 54122291 | A2 | 19790921 | JP 1979-21790 | 19790226 |
| JP 60058237 | B4 | 19851219 | | |
| CA 1132539 | A1 | 19820928 | CA 1979-322301 | 19790226 |
| AT 8003862 | A | 19810415 | AT 1980-3862 | 19800725 |
| US 31926 | E | 19850625 | US 1982-420804 | 19820921 |

PRIORITY APPLN. INFO.:

| | |
|---|---|
| DE 1978-2808153 | 19780225 |
| DE 1978-2851226 | 19781127 |
| DE 1978-2851270 | 19781127 |
| US 1979-13006 | 19790221 |

GI




I

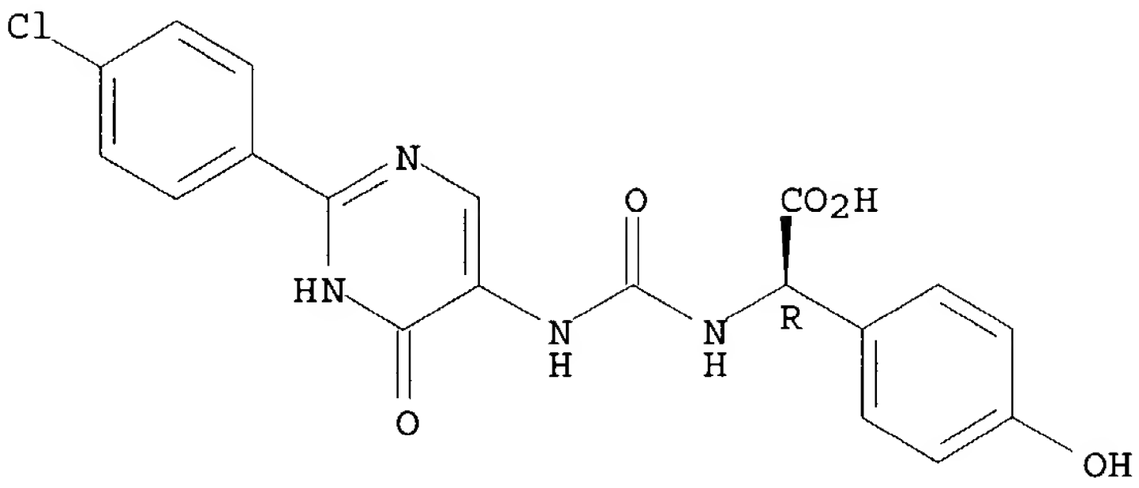
AB The penicillins I (R = optionally substituted Ph; R1 = Ph, 4-HOC6H4, 1,4-cyclohexadienyl; n = 0, 1) were prepared Thus 4-ClC6H4CH2C(:NH)NH2 was condensed with EtO2CNHC(:CHONa)CO2Et to give 42.5% 5-amino-2-p-chlorobenzyl-4-pyrimidinol which was treated with COCl2 and amoxycillin-3H2O to give 73% I (R = 4-ClC6H4, R1 = 4-HOC6H4, n = 1) as the Na salt.

IT **75424-41-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of aminopenicillanic acid by)

RN 75424-41-8 CAPLUS

CN Benzeneacetic acid, α-[[[[2-(4-chlorophenyl)-1,4-dihydro-4-oxo-5-pyrimidinyl]amino]carbonyl]amino]-4-hydroxy-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




L10 ANSWER 42 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1980:41984 CAPLUS
DOCUMENT NUMBER: 92:41984
TITLE: 2-Phenyl-4-hydroxy-6-methylpyrrolo[3,2-d]pyrimidine
INVENTOR(S): Sokolova, V. N.; Novitskii, K. Yu.
PATENT ASSIGNEE(S): Ordzhonikidze, S., All-Union Scientific-Research Chemical-Pharmaceutical Institute, USSR
SOURCE: U.S.S.R. From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1979, (37), 90.
CODEN: URXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

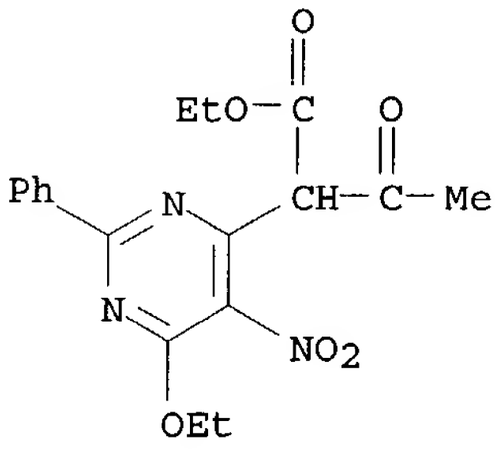
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| SU 690016 | T | 19791005 | SU 1977-2521258 | 19770803 |

PRIORITY APPLN. INFO.: SU 1977-2521258 19770803

AB Title compound was prepared by reacting 2-phenyl-4-ethoxy-5-nitro-6-[1-(ethoxycarbonyl)-2-oxopropyl]pyrimidine with Zn in HOAc at 60-90° followed by refluxing the resulting 2-phenyl-4-ethoxy-6-methyl-7-(ethoxycarbonyl)pyrrolo[3,2-d]pyrimidine with HCl.

IT **72168-65-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive cyclization of)

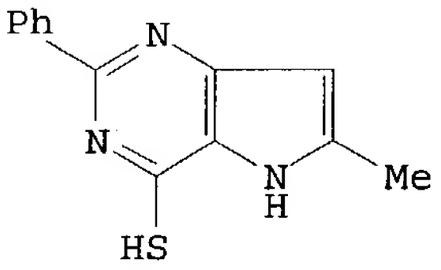
RN 72168-65-1 CAPLUS
CN 4-Pyrimidineacetic acid, α-acetyl-6-ethoxy-5-nitro-2-phenyl-, ethyl ester (9CI) (CA INDEX NAME)




L10 ANSWER 43 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1980:15521 CAPLUS
DOCUMENT NUMBER: 92:15521
TITLE: Study of pyrrolo[3,2-d]pyrimidine. III

09/ 811,359

AUTHOR(S): Sokolova, V. N.; Modnikova, G. A.; Novitskii, K. Yu.; Kravchenko, A. I.; Chernov, V. A.; Shcherbakova, L. I.; Pershin, G. N.
CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1979), 13(9), 17-22
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 92:15521
GI



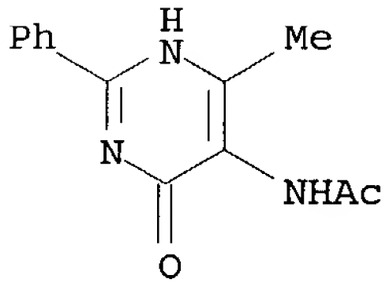

I

AB 2-Phenyl-4-mercapto-6-methylpyrrolo[3,2-d]pyrimidine (I) [72168-74-2] inhibited growth of Lactobacillus casei in vitro at 1-10 μg/mL and of Mycobacterium tuberculosis at 4 μg/mL. In expts. in vivo, I was active against sarcoma in mice and rats, but not against leukemia in mice. The other 6 4-alkylamino-2-phenyl-6-methylpyrrolo[3,2-d]pyrmidines and 11 4-alkyl(aralkyl)thio-2-phenyl-6-methylpyrrolo[3,2-d]pyrimidines prepared and tested showed no antibacterial activity, with the exception of 4-isobutylamino-2-phenyl-6-methylpyrrolo[3,2-d]pyrimidine [72168-70-8] which was weakly active.

IT **72168-63-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

RN 72168-63-9 CAPLUS

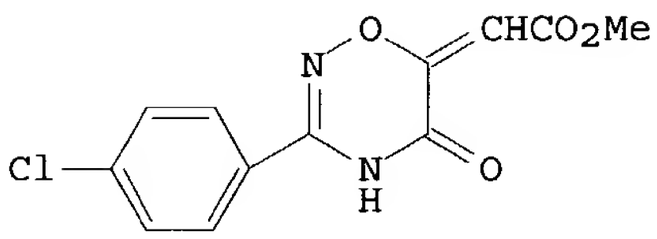
CN Acetamide, N-(1,4-dihydro-6-methyl-4-oxo-2-phenyl-5-pyrimidinyl)- (9CI) (CA INDEX NAME)




L10 ANSWER 44 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1979:420462 CAPLUS
DOCUMENT NUMBER: 91:20462
TITLE: Synthesis of 1,2,4-oxadiazines and their rearrangement to pyrimidines
AUTHOR(S): Santilli, Arthur A.; Scotese, Anthony C.
CORPORATE SOURCE: Res. Dev. Div., Wyeth Lab., Inc., Radnor, PA, 19087, USA
SOURCE: Journal of Heterocyclic Chemistry (1979), 16(2), 213-16
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English

09/ 811,359

OTHER SOURCE(S): CASREACT 91:20462
GI



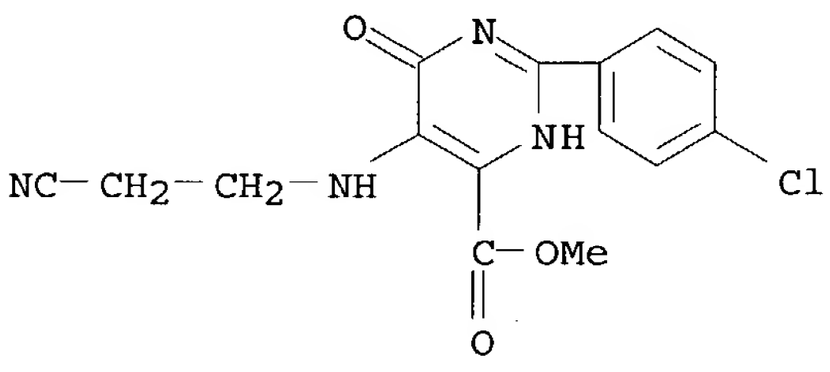
I

AB Several amide oximes underwent condensation reactions with MeO2CC.tplbond.CCO2Me to give 1:1 adducts. Under basic conditions, these adducts underwent ring closure to give several Me [3-(substituted)-4,5-dihydro-5-oxo-6H-1,2,4-oxadiazin-6-ylidene]acetates, e.g. I. The reactions of these compds. with a variety of amines resulted in addition-rearrangement reactions with the formation of the corresponding Me 2-substituted-5-substituted amino-1,6-dihydro-6-oxo-4-pyrimidinecarboxylates.

IT **70274-26-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 70274-26-9 CAPLUS

CN 4-Pyrimidinecarboxylic acid, 2-(4-chlorophenyl)-5-[(2-cyanoethyl)amino]-1,6-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)



L10 ANSWER 45 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1979:49472 CAPLUS

DOCUMENT NUMBER: 90:49472

TITLE: Relation between the chemical structure and stimulating activity of some nitro-, hydroxy-, and amino-substituted pyrimidines as illustrated by mono- and dicotyledonous plants

AUTHOR(S): Vladimirtsev, I. F.; Borisenko, V. P.; Boldyrev, I. V.; Nasyr, I. A.

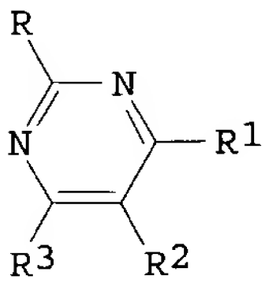
CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR

SOURCE: Fiziologicheski Aktivnye Veshchestva (1978), 10, 45-7
CODEN: FAVUAI; ISSN: 0533-1153

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI



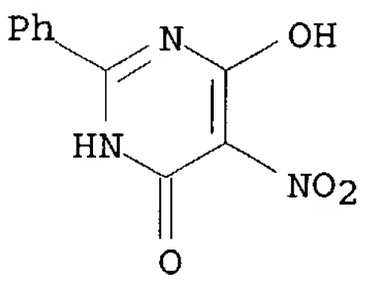
I

AB Of 17 title compds. I (R = H, Me, Ph, OH, or NH2; R1 = H, Cl, or OH; R2 = NH2, H, NO2, NHCOCO2Et, or NHAc; R3 = H, OH, or Me) 5-aminopyrimidine [591-55-9] and 4-methyl-6-hydroxypyrimidine [3524-87-6] most effectively stimulated the growth of lettuce and oats. Synthesis was given.

IT **68905-99-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and plant-growth stimulating activity of)

RN 68905-99-7 CAPLUS

CN 4(1H)-Pyrimidinone, 6-hydroxy-5-nitro-2-phenyl- (9CI) (CA INDEX NAME)

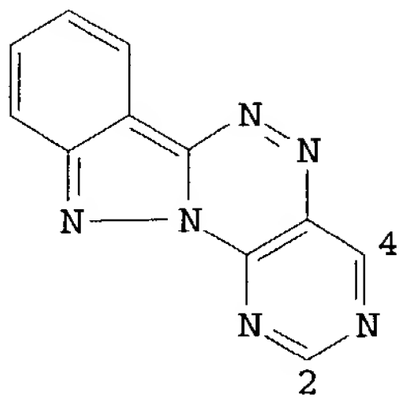


L10 ANSWER 46 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

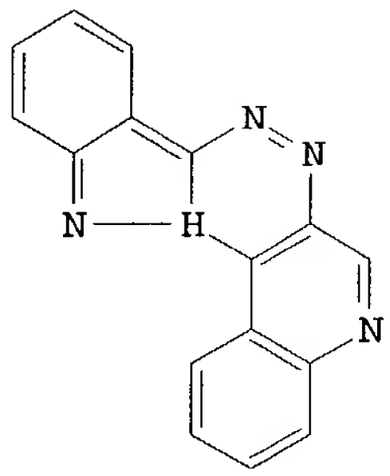
ACCESSION NUMBER: 1979:7589 CAPLUS
DOCUMENT NUMBER: 90:7589
TITLE: Polycyclic compounds
INVENTOR(S): Dunkelmann, Guenter
PATENT ASSIGNEE(S): BASF A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 27 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 2707710 | A1 | 19780824 | DE 1977-2707710 | 19770223 |
| GB 1596690 | A | 19810826 | GB 1978-7022 | 19780222 |
| JP 54060328 | A2 | 19790515 | JP 1978-19179 | 19780223 |

PRIORITY APPLN. INFO.: DE 1977-2707710 19770223
GI



I



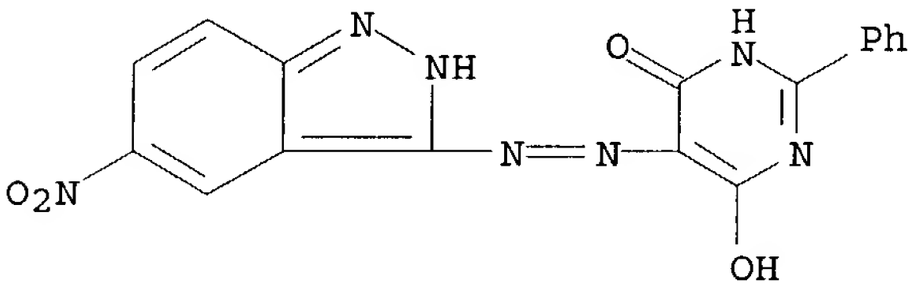
II

AB Polycyclic dyes containing substituted I and II nuclei were prepared and used to dye polyester fiber and PVC [9002-86-2] fast yellow shades. Thus, 3-aminoindazole → 2-phenyl-4,6-dihydroxypyrimidine [**68386-19-6**] was cyclized by heating in HOAc containing H2SO4 to give I(2-Ph, 4-OH) [68386-18-5]. The other I and II were similarly prepared

IT **68386-06-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)

RN 68386-06-1 CAPLUS

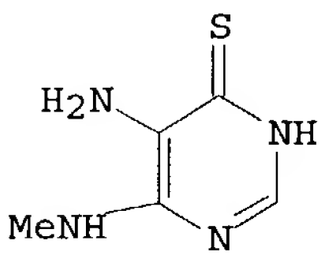
CN 4(1H)-Pyrimidinone, 6-hydroxy-5-[(5-nitro-2H-indazol-3-yl)azo]-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 47 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:78554 CAPLUS
DOCUMENT NUMBER: 86:78554
TITLE: Hair dyeing agent
INVENTOR(S): Kubersky, Hans P.
PATENT ASSIGNEE(S): Henkel und Cie. G.m.b.H., Fed. Rep. Ger.
SOURCE: Ger. Offen., 13 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 2523045 | A1 | 19761202 | DE 1975-2523045 | 19750524 |

PRIORITY APPLN. INFO.: DE 1975-2523045 19750524
GI



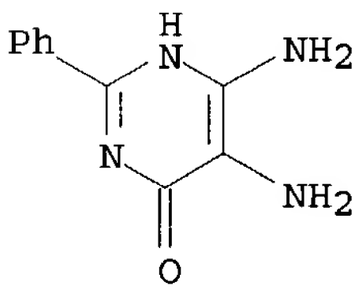
I

AB Diaminopyrimidine derivs. are developer components for oxidative dyeing of hair which provide a wide range of color nuances, are water soluble, are toxicol. and dermatol. innocuous, and have good fastness. For example, a dye cream was prepared containing (I) [61595-49-1] as developer and m-diaminoanisole as coupler. Gray hair treated with this cream developed an orange-brown color when oxidized with air and a brown color when oxidized with 1° H2O2.

IT **61595-45-7**
RL: BIOL (Biological study)
(as dye, for hair)

RN 61595-45-7 CAPLUS

CN 4(1H)-Pyrimidinone, 5,6-diamino-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 48 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1977:55486 CAPLUS
DOCUMENT NUMBER: 86:55486
TITLE: Azapurinones
INVENTOR(S): Broughton, Barbara J.; Large, Bryan J.; Marshall, Stuart Malcolm; Pain, David L.; Wooldridge, Kenneth R. H.
PATENT ASSIGNEE(S): May and Baker Ltd., UK
SOURCE: Ger. Offen., 34 pp. Addn. to Ger. Offen. 2,162,096.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

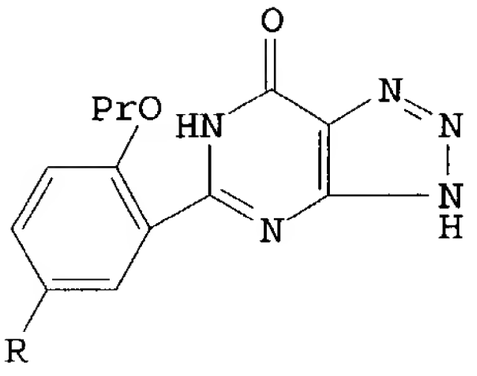
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 2618694 | A1 | 19761111 | DE 1976-2618694 | 19760428 |
| GB 1493685 | A | 19771130 | GB 1975-17573 | 19750428 |
| US 4039544 | A | 19770802 | US 1976-680444 | 19760426 |
| BE 841181 | A4 | 19761027 | BE 1976-166501 | 19760427 |
| ZA 7602489 | A | 19770427 | ZA 1976-2489 | 19760427 |
| CA 1077933 | A1 | 19800520 | CA 1976-251095 | 19760427 |
| NL 7604548 | A | 19761101 | NL 1976-4548 | 19760428 |

PRIORITY APPLN. INFO.:

| | |
|---|---|
| GB 1975-17573 | 19750428 |
| GB 1975-23785 | 19750602 |
| GB 1970-59552 | 19701215 |
| GB 1970-59556 | 19701215 |
| GB 1971-49756 | 19711026 |

| | | |
|---|---|---|
| GB | 1971-53457 | 19711117 |
| US | 1971-207986 | 19711214 |
| US | 1973-364425 | 19730529 |

GI



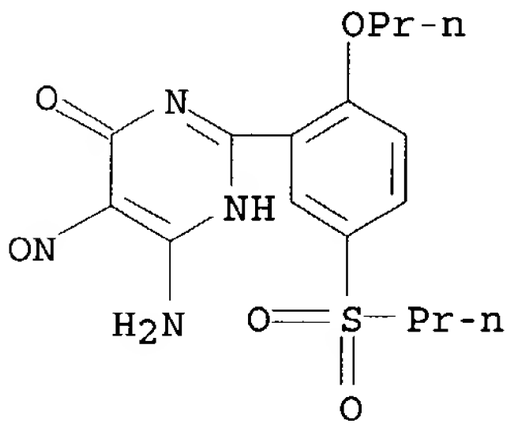
I

AB 3,6-Dihydro-7H-v-triazolo[4,5-d]pyrimidin-7-ones (I; R = MeO2C, EtO2C, BuO2C, BuS, BuSO, MeSO2, PrSO2, Me2CHSO2, BuSO2, Me2CHCH2SO2), useful in treatment of bronchial asthma (no data), are prepared by reaction of 5,6-diamino-2-phenyl-4(3H)-pyrimidinones with HNO2. The diaminopyrimidinones are obtained from 5-nitroso-6-aminopyrimidinones which are prepared from the 2-propoxybenzamides via the benzamidines. Thus, reaction of 15 % 5,6-diamino-2-[2-propoxy-5-(propylsulfonyl)phenyl]-4(3H)-pyrimidinone with NaNO2 in aqueous HCl at 0°, followed by stirring 2 hr at 0° and 18 hr at room temperature, gives 12 g I (R = PrSO2).

IT **61627-25-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, and diaminopyrimidinone from)

RN 61627-25-6 CAPLUS

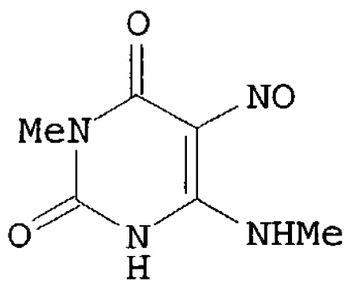
CN 4(1H)-Pyrimidinone, 6-amino-5-nitroso-2-[2-propoxy-5-(propylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

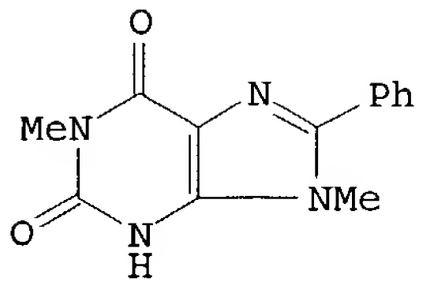


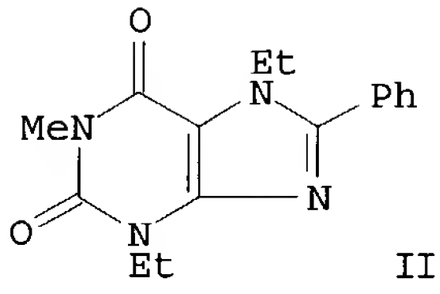
L10 ANSWER 49 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

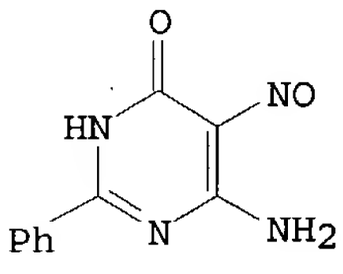
| | |
|---|---|
| ACCESSION NUMBER: | 1977:5410 CAPLUS |
| DOCUMENT NUMBER: | 86:5410 |
| TITLE: | A new, general synthesis of purines |
| AUTHOR(S): | Yoneda, Fumio; Nagamatsu, Tomohisa |
| CORPORATE SOURCE: | Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, Japan |
| SOURCE: | Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1976), (14), 1547-50<br>CODEN: JCPRB4; ISSN: 0300-922X |
| DOCUMENT TYPE: | Journal |
| LANGUAGE: | English |
| OTHER SOURCE(S): | CASREACT 86:5410 |

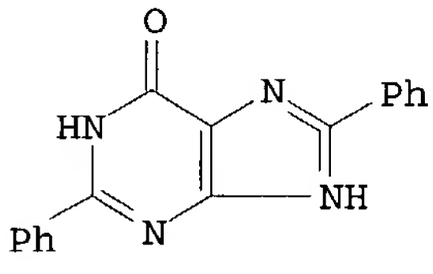
GI


I


II


III


IV

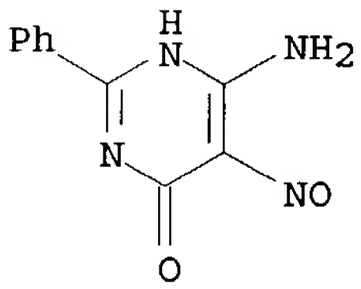

V

AB 6-Amino-5-nitrosouracil derivs. underwent cyclocondensation reactions with RCH:NNMe2, prepared in situ by reaction of RCHO with NH2NMe2, to give the corresponding xanthine derivs. Thus, the uracil I with PhCH:NNMe2 in DMF gave 71% II. Alkylation of 9-substituted 1-methylxanthines with excess alkyl halide in DMF in the presence of K2CO3 gave the corresponding 3,7-dialkyl-1-methylxanthine, with elimination of the 9-substituent. Thus, II with EtI and K2CO3 in DMF gave 68% III. Similar treatment of 6-amino-4-hydroxy-5-nitroso-2-phenylpyrimidines with RCH:NNMe2 gave the corresponding purines. Thus, the pyrimidine IV with PhCH:NNMe2 in DMF gave 49% purine V.

IT **5466-66-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction with benzaldehyde dimethylhydrazone)

RN 5466-66-0 CAPLUS

CN 4(1H)-Pyrimidinone, 6-amino-5-nitroso-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 50 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:572422 CAPLUS
DOCUMENT NUMBER: 83:172422
TITLE: Antiallergic activity of 2-phenyl-8-azapurin-6-ones
AUTHOR(S): Broughton, B. J.; Chaplen, P.; Knowles, P.; Lunt, E.; Marshall, S. M.; Pain, D. L.; Wooldridge, K. R. H.
CORPORATE SOURCE: Res. Lab., May and Baker Ltd., Dagenham/Essex, UK
SOURCE: Journal of Medicinal Chemistry (1975), 18(11), 1117-22
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 83:172422

GI For diagram(s), see printed CA Issue.

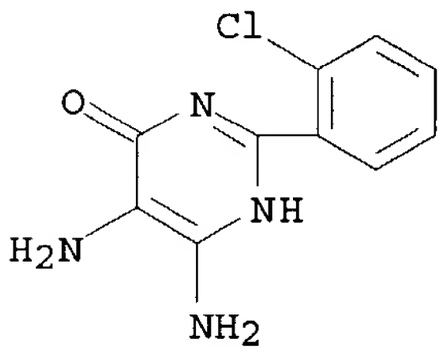
AB The cycloaddn. reaction of benzamidines with Et cyanonitrosoacetate [5457-25-0] gave aminophenylnitrosopyrimidinones which underwent reduction, nitrosation, and cyclization to give 44 title azapurinones. The azapurinones had varying antiallergic activity in the rat passive cutaneous anaphylactic reaction with 2-(o-propoxyphenyl)-8-azapurin-6-one (I) [37762-06-4] being 40 times more potent than disodium cromoglycate

[15826-37-6]. Structure activity relations were discussed.

IT **57075-30-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cycloaddn. with sodium nitrate)

RN 57075-30-6 CAPLUS

CN 4(1H)-Pyrimidinone, 5,6-diamino-2-(2-chlorophenyl)- (9CI) (CA INDEX NAME)




L10 ANSWER 51 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1974:505449 CAPLUS

DOCUMENT NUMBER: 81:105449

TITLE: Novel synthetic route to heterocycles via intramolecular cycloaddition of azalogs of hexatriene. New syntheses of purines and pyrazolo[3,4-d]pyrimidines

AUTHOR(S): Yoneda, Fumio; Higuchi, Masatsugu; Nagamatsu, Tomohisa

CORPORATE SOURCE: Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, Japan

SOURCE: Journal of the American Chemical Society (1974), 96(17), 5607-8
CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

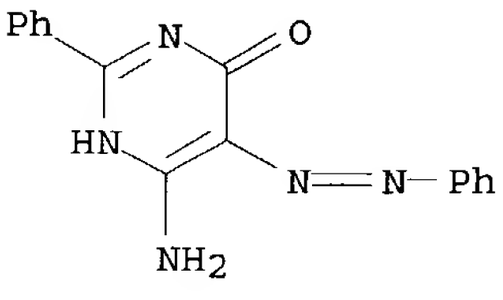
GI For diagram(s), see printed CA Issue.

AB The thermolysis of 5-(arylazo)-1,3-dimethyl-6-[[(dimethylamino)methylene]amino]-uracils gave 8-(dimethylamino)theophylline and 5-aryl-1,3-dimethyl-7-(dimethylamino)-5,6(or 5,8)-dihydro-6-azalumazines. The reaction of 6-amino-1,3-dimethyl-5-(phenylazo)uracil with aromatic aldehydes gave the corresponding 8-aryltheophyllines and 5-aryl-1,3-dimethyl-7-phenyl-5,6(or 5,8)-dihydro-6-azalumazines. This purine synthesis is applicable to other 6-amino-5-(phenylazo)pyrimidines such as 6-amino-1-methyl-5-(phenylazo)uracil and 6-amino-4-hydroxy-2-phenyl-5-(phenylazo)pyrimidine to give the resp. purine derivs. Heating 6-(benzylidene-hydrazino)uracil derivs. with aromatic aldehydes in DMF gave the corresponding 3-aryl-2-benzylpyrazolo[3,4-d] pyrimidine-4,6(5H,-7H)-diones I in excellent yields.

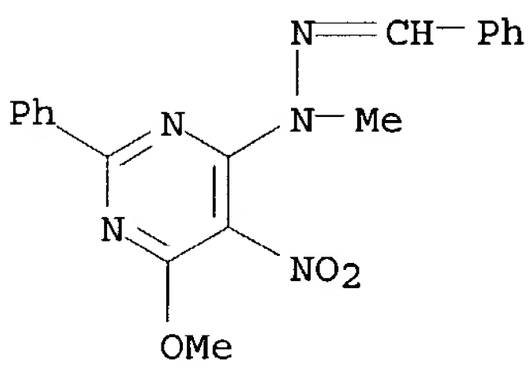
IT **54014-72-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation with aromatic aldehydes)

RN 54014-72-1 CAPLUS

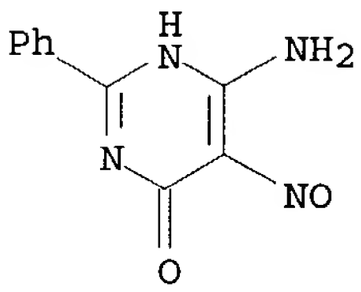
CN 4(1H)-Pyrimidinone, 6-amino-2-phenyl-5-(phenylazo)- (9CI) (CA INDEX NAME)



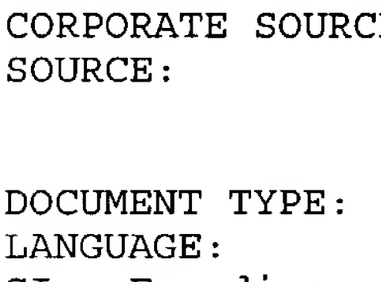
L10 ANSWER 52 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1974:477865 CAPLUS
DOCUMENT NUMBER: 81:77865
TITLE: Photochemical synthesis of condensed triazole N-oxide
AUTHOR(S): Maki, Yoshifumi; Suzuki, Mikio; Izuta, Keiji; Iwai, Shunji
CORPORATE SOURCE: Gifu Coll. Pharm., Gifu, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1974), 22(6), 1269-74
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Photolysis of the uracil I (R = H) in C6H6 gave the pyrazolopyrimidine II and the triazolopyrimidine oxide III. Photolysis of I (R = Me) in MeCN at 338 mμ gave III exclusively.
IT **53246-62-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(photolysis of)
RN 53246-62-1 CAPLUS
CN Benzaldehyde, (6-methoxy-5-nitro-2-phenyl-4-pyrimidinyl)methylhydrazone (9CI) (CA INDEX NAME)




L10 ANSWER 53 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1973:466312 CAPLUS
DOCUMENT NUMBER: 79:66312
TITLE: New synthesis of substituted 8-aminopurine derivatives
AUTHOR(S): Yoneda, Fumio; Higuchi, Masatsugu; Matsumura, Takafumi; Senga, Keitaro
CORPORATE SOURCE: Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1973), 46(6), 1836-9
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The treatment of 6-amino-5-nitrosopyrimidinediones with Vilsmeier-type reagents (substituted formamides and phosphorus oxychloride) afforded substituted 8-aminopurines (I, R = NMe2, NEt2, NHMe, NMePh). However, the treatment of 6-amino-4-hydroxy-2-methyl-5-nitrosopyrimidine with the same reagents gave 2-(chloromethyl)-8-(dimethylamino)-6-hydroxypurine.
IT **5466-66-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with formamides)
RN 5466-66-0 CAPLUS
CN 4(1H)-Pyrimidinone, 6-amino-5-nitroso-2-phenyl- (9CI) (CA INDEX NAME)

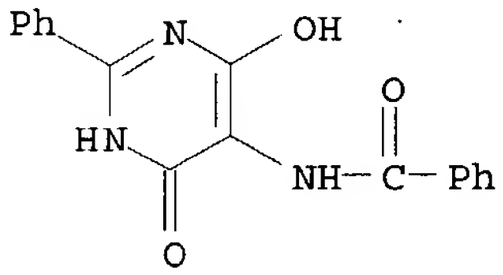


L10 ANSWER 54 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1972:539952 CAPLUS
DOCUMENT NUMBER: 77:139952
TITLE: Formation of new mesoionic pyrimidines
AUTHOR(S): Maki, Y.; Sako, M.; Suzuki, M.
CORPORATE SOURCE: Gifu Coll. Pharm., Gifu, Japan
SOURCE: Journal of the Chemical Society, Chemical Communications (1972), (17), 999-1000
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Pyrolysis of 4,6-dimethoxy-5-nitropyrimidine (I) at 200° for 15 min gave 70% anhydro-4-hydroxy-1,3-dimethyl-5-nitro-6-oxopyrimidinium (II) hydrochloride and 1-methyl-4-methoxy-5-nitro-6(1H)-pyrimidinone which at 200° gave II. Similarly the 2-phenyl derivative of I gave the corresponding pyrimidinium (III) hydrochloride (80%) and pyrimidinone which at 200° gave III. II or III with boiling aqueous KOH gave MeHNCOC(NO2):C(OH)NHMe quant. Pyrolysis of 4,6-dimethoxy-2-phenylpyrimidine caused O → N alkyl migration to give the correspondlng N-alkyl derivs.
IT **29939-35-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prolysis of)
RN 29939-35-3 CAPLUS
CN Pyrimidine, 4,6-dimethoxy-5-nitro-2-phenyl- (8CI, 9CI) (CA INDEX NAME)

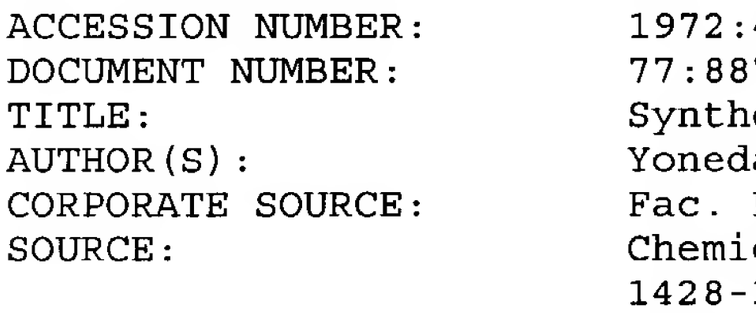


L10 ANSWER 55 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1972:501508 CAPLUS
DOCUMENT NUMBER: 77:101508
TITLE: Structure of aroyl isocyanide trimers
AUTHOR(S): Dounchis, Harry
CORPORATE SOURCE: Chem. Res. Dev. Cent., FMC Corp., Princeton, NJ, USA
SOURCE: Journal of Organic Chemistry (1972), 37(16), 2583-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The structure of the trimer of benzoyl isocyanide, prepared by the action of AgCN on BzBr, is 7-benzoylimino-2,5-diphenyloxazolo[5,4-d]pyrimidin-7-one. The scope and limitation of the trimerization reaction is discussed.
IT **34906-02-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
RN 34906-02-0 CAPLUS
CN Benzamide, N-(1,4-dihydro-6-hydroxy-4-oxo-2-phenyl-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 56 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1972:488766 CAPLUS
DOCUMENT NUMBER: 77:88766
TITLE: Syntheses of some androstano[2,3-g]pteridines
AUTHOR(S): Yoneda, Fumio; Fukazawa, Shinobu; Nishigaki, Sadao
CORPORATE SOURCE: Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1972), 20(7), 1428-31
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Morpholino and pyrrolidino derivs. of 17β-hydroxy-5α-androstan-3-one reacted with 6-amino-5-nitrosopyrimidines or 6-amino-5-phenylazo-pyrimidines to give the corresponding androstano [2,3-g] pteridines. These steroidal pteridines were also prepared by the Isay pteridine synthesis from 17β-hydroxy-5α-androstane-2,3-dione and the corresponding 5,6-diaminopyrimidines.
IT **38522-17-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 38522-17-7 CAPLUS
CN 4(1H)-Pyrimidinone, 6-amino-5-[(4-nitrophenyl)azo]-2-phenyl- (9CI) (CA INDEX NAME)



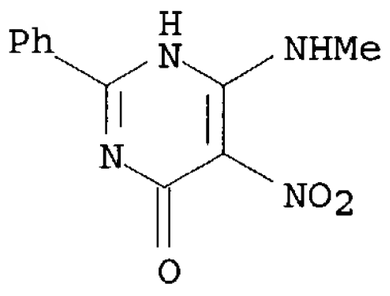
L10 ANSWER 57 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1972:46170 CAPLUS
DOCUMENT NUMBER: 76:46170
TITLE: Pteridines. XXVI. Preparation and properties of some 3,4- and 5,6-dihydropteridines
AUTHOR(S): Taylor, Edward C.; Thompson, Malcolm J.; Perlman, Katherine; Mengel, Rudolf; Pfleiderer, Wolfgang
CORPORATE SOURCE: Dep. Chem., Princeton Univ., Princeton, NJ, USA
SOURCE: Journal of Organic Chemistry (1971), 36(26), 4012-25
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Treatment of 8-alkyl-7(8H)-pteridinone-6-carboxylic acid derivs.

(substituted at position 4 with H or Me) with NaBH4 gives bright yellow dihydro compds. which are 10,000 times weaker acids, and exhibit uv absorption maxima some 50-60 nm higher, than the starting pteridinones. The influence of 2 and 4-substituents on this reduction was carefully examined, and evaluation of both spectroscopic (uv. ir, and NMR) and chemical data has shown that these reduction products are 3,4-dihydro derivs., and not 4,8- (or 5,8-) dihydro derivs. as previously suggested. By contrast, catalytic reduction of the same series of 8-alkyl-7(8H)-pteridinone-6-carboxylic acids and esters gave 5,6-dihydro compds. with different chemical and phys. properties. 3,4-Dihydro compds. rearrange quant. and irreversibly to the 5,6-dihydro isomers in F3CCO2H.

IT **31937-03-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 31937-03-8 CAPLUS

CN 4(1H)-Pyrimidinone, 6-(methylamino)-5-nitro-2-phenyl- (9CI) (CA INDEX NAME)




L10 ANSWER 58 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1971:510265 CAPLUS

DOCUMENT NUMBER: 75:110265

TITLE: Reaction of 4,6-dimethoxy-5-nitropyrimidine with methylhydrazine. Formation of 4-hydrazine-6-hydroxypyrimidine

AUTHOR(S): Christensen, Bert E.; Stahl, Quade; Lehmkuhl, Frank

CORPORATE SOURCE: Dep. Chem., Oregon State Univ., Corvallis, OR, USA

SOURCE: Journal of Organic Chemistry (1971), 36(17), 2462-6
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 75:110265

AB Reaction of 4,6-dimethoxy-5-nitropyrimidine (I) with MeNHNH2 in refluxing pyridine or BuOH involves methylation of the solvent by I and the nucleophilic substitution and demethylation of the methylhydrazino substituent in the 5 position to yield 4-hydrazino-6-hydroxypyrimidine. The first step in this sequence of reactions involves the methylation of the solvent, followed by nucleophilic substitution of methylhydrazine in the 4 position, migration of its Me substituent to form C to O bond with the adjacent nitro substituent, and eventual elimination of Me nitrite from the 5 position as one of the reaction products. 4,6-Dimethoxy-5-nitropyrimidine reacts with pyridine (in the absence of MeNHNH2) to yield an insol. methylpyridium salt which is not a precursor of 4-hydrazino-6-hydroxypyrimidine. The mother liquor from this reaction on acid hydrolysis yields 4-hydroxy-6-methoxy-5-nitropyrimidine and reacts with MeNHNH2 to yield 4-hydroxy-6-hydrazinopyrimidine. Both 4-chloro-6-hydroxy-5-nitropyrimidine and 4,6-dichloro-5-nitropyrimidine react with MeNHNH2 in alc. to yield the corresponding methylhydrazino derivs.

IT **29939-35-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 29939-35-3 CAPLUS

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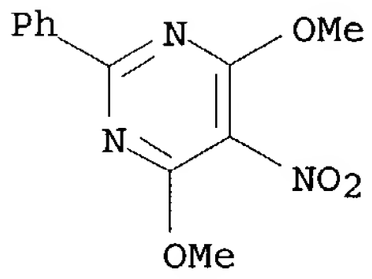
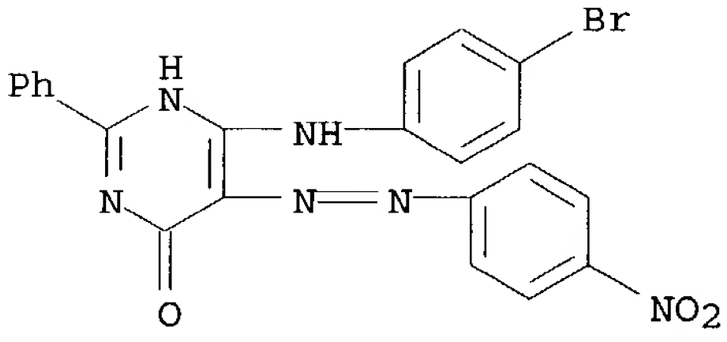
CN Pyrimidine, 4,6-dimethoxy-5-nitro-2-phenyl- (8CI, 9CI) (CA INDEX NAME)




L10 ANSWER 59 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1971:112015 CAPLUS
DOCUMENT NUMBER: 74:112015
TITLE: New synthesis of alloxazines
AUTHOR(S): Yoneda, Fumio; Ichiba, Misuzu; Ogiwara, Kazuko; Nishigaki, Sadao
CORPORATE SOURCE: Sch. Med., Keio Univ., Tokyo, Japan
SOURCE: Journal of the Chemical Society [Section] D: Chemical Communications (1971), (1), 23
CODEN: CCJDAO; ISSN: 0577-6171
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB 2-Phenyl-2-deoxyalloxazine (I, R = H) and its 7-chloro (I, R = Cl) and 7-bromo derivative (I, R = Br) were prepared by cyclization of II (R = H, Cl, Br) with 10% H2SO4 in HOAc. Using 20% H2SO4, HOAc alone, or F3CCO2H alone did not lead to cyclization. 5-Chlorophenylazo- and 5-phenylazo-6-anilino-4-hydroxy-2-phenylpyrimidine could not be cyclized by this method. II were prepared by treating 6-amino-2-phenyl-4-hydroxypyrimidine with p-RC6H4NH2 and then coupling with p-nitrobenzenediazonium chloride.
IT **31595-55-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 31595-55-8 CAPLUS
CN 4(3H)-Pyrimidinone, 6-(p-bromoanilino)-5-[(p-nitrophenyl)azo]-2-phenyl- (8CI) (CA INDEX NAME)




L10 ANSWER 60 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1971:111997 CAPLUS
DOCUMENT NUMBER: 74:111997
TITLE: Oxidation of 5-nitrosopyrimidines by nitrous acid. A synthesis of 5-nitropyrimidines
AUTHOR(S): Nishigaki, Sadao; Ogiwara, Kazuko; Yoneda, Fumio
CORPORATE SOURCE: Sch. Med., Keio Univ., Tokyo, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1971), 19(2), 418-19
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English

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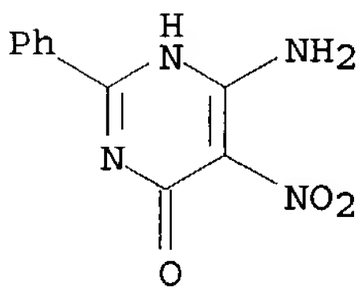
AB Some 2,4,6-trisubstituted pyrimidines gave with NaNO2 in H2SO4 the corresponding 5-nitropyrimidines, by way of nitrosation. Thus, 2-phenyl-4-hydroxy-6-morpholinopyrimidine gave 2-phenyl-4-hydroxy-5-nitro-6-morpholinopyrimidine.

IT **23120-15-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 23120-15-2 CAPLUS

CN 4-Pyrimidinol, 6-amino-5-nitro-2-phenyl- (8CI) (CA INDEX NAME)




L10 ANSWER 61 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1969:449899 CAPLUS
DOCUMENT NUMBER: 71:49899
TITLE: Heterocyclic studies. VIII. 2-Phenylpteridine and some related compounds
AUTHOR(S): Clark, Jim; Murdoch, P. N. T.; Roberts, D. L.
CORPORATE SOURCE: Univ. Salford, Salford, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1969), (10), 1408-12
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English

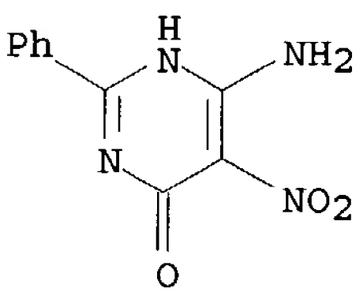
GI For diagram(s), see printed CA Issue.

AB Syntheses of 2-phenylpteridine (I) and its 4- and 7-monomethyl, 4,7- and 6,7-dimethyl, and 4,6,7-trimethyl derivs. are described. Oxidation of 2-phenyl-, 7-methyl-2-phenyl-, and 6,7-dimethyl-2-phenylpteridines with H2O2 in acetic acid gave the corresponding 4-hydroxy derivs. Further oxidation of 4-hydroxy-2-phenylpteridine gave 4,6,7-trihydroxy-2-phenylpteridine. In acid solution, 2-phenylpteridine gave a mixture of 3,4-monohydrated and 5,6,7,8-dihydrated cations which rapidly changed to a solution almost free of the monohydrate. 4-Methyl- and 4,7-dimethyl-2-phenylpteridines also gave essentially all 5,6,7,8-dihydrated cations but mainly 3,4-hydrated species were present in the equilibrium mixts. of cations formed from 7-methyl- and 6,7-dimethyl-2-phenylpteridine. 1H N.M.R. and uv spectra and pKa values are recorded.

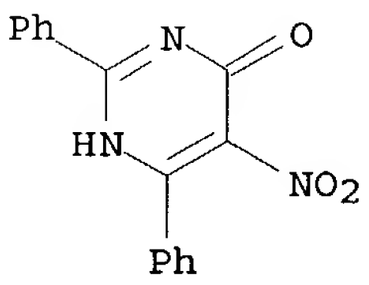
IT **23120-15-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 23120-15-2 CAPLUS

CN 4-Pyrimidinol, 6-amino-5-nitro-2-phenyl- (8CI) (CA INDEX NAME)



L10 ANSWER 62 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1969:11661 CAPLUS
DOCUMENT NUMBER: 70:11661
TITLE: Syntheses of 4,5-disubstituted 2,6-diarylpyrimidines
AUTHOR(S): Weidinger, Hans; Sturm, Hans Juergen
CORPORATE SOURCE: Farbenforschungslab., Bad. Anilin- und Soda-Fabrik A.-G., Ludwigshafen/Rhein, Fed. Rep. Ger.
SOURCE: Justus Liebigs Annalen der Chemie (1968), 716, 143-6
CODEN: JLACBF; ISSN: 0075-4617
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 70:11661
AB RCN reacted with SO3 to give 4,6-bis(R-substituted)-1,2,3,5-oxathiadiazine 2,2-dioxides (I), which lose SO2 and add 2C fragments to give 2,6-bis(R-substituted)-4-(R1-substituted)-5-(R2-substituted)-pyrimidines (II). Reaction of I with AcCH2CO2Et gave II (R = Ph, R1 = OH, R2 = CO2Et); treatment of I with CH2(CN)CO2Et gave II (R = Ph, R1 = OH, R2 = CN); CH2(CN)2 and I gave II (R = Ph or p-MeC6H4, R1 = NH2, R2 = CN), while 1-morpholinocyclohexene led to 2,4-diphenyl-5,6,7,8-tetrahydro-quinazoline.
IT **20954-88-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 20954-88-5 CAPLUS
CN 4-Pyrimidinol, 5-nitro-2,6-diphenyl- (8CI) (CA INDEX NAME)




L10 ANSWER 63 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1968:49645 CAPLUS
DOCUMENT NUMBER: 68:49645
TITLE: 4-Amino-5-arylazopyrimidine derivatives
INVENTOR(S): Fujimoto, Yasuo; Teranishi, Masayuki
PATENT ASSIGNEE(S): Kyowa Fermentation Industry Co., Ltd.
SOURCE: Jpn. Tokkyo Koho, 4 pp.
CODEN: JAXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 42008388 | B4 | 19670411 | JP | 19631228 |

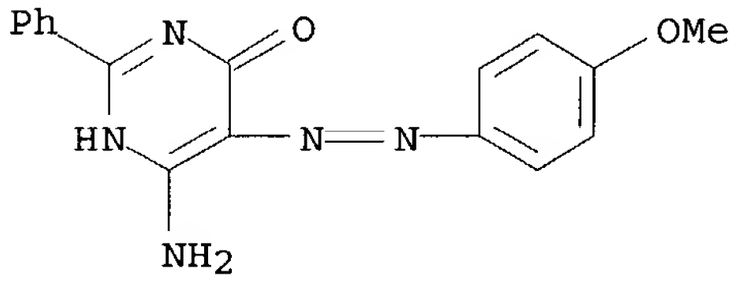
AB A mixture of 4.35 g. Et 2-phenylazocyanoacetate, 80 ml. EtOH, 0.42 g. Na, and 1.55 g. thiourea is refluxed 2 hrs., cooled, and neutralized with AcOH and the product recrystd. (EtOH-pyridine) to give 3.5 g. 2-mercapto-4-amino-5 - phenylazo - 6 - pyrimidinol. Similarly prepared are 4-amino-2,6-dihydroxy-5-(p-hydroxyphenylazo)pyrimidine, 2,4-diamino-5-(p-methylphenylazo)-6-hydroxypyrimidine, 4-amino-5-(m-nitrophenylazo)-6-hydroxy-2-methylpyrimidine, 4-amino - 6-hydroxy-5 - phenylazo - 2 - (methylthio)pyrimidine, 4 - amino - 5-phenylazo-6-hydroxypyridine, 4-amino-6-hydroxy-2-phenyl-5-(p-methoxyphenylazo)pyridine, 4-amino-2-(p-chlorophenyl) - 6-hydroxy - 5 - (m-carboxyphenylazo)pyrimidine, 4 - amino - 6 - hydroxy-5-(p-

sulfophenylazo)-2-(methylthio)pyrimidine, 4-amino-2-ethoxy-6-hydroxy-5-(o-chlorophenylazo)pyrimidine, 4-amino-6-hydroxy-2-pyridyl- 5 - (m - methylphenylazo) - 1 - methylpyrimidine, and 4-amino-6-hydroxy-5-(p-nitrophenylazo)-2-benzylpyrimidine. The products are intermediates for the manufacture of condiments and pharmaceuticals.

IT **17041-99-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 17041-99-5 CAPLUS

CN 4-Pyrimidinol, 6-amino-5-[(p-methoxyphenyl)azo]-2-phenyl- (8CI) (CA INDEX NAME)




L10 ANSWER 64 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1965:9095 CAPLUS

DOCUMENT NUMBER: 62:9095

ORIGINAL REFERENCE NO.: 62:1651d-e

TITLE: Syntheses of 4-hydroxy-5-nitropyrimidines

AUTHOR(S): Simchen, G.

CORPORATE SOURCE: Tech. Hochschule, Stuttgart, Germany

SOURCE: Angew. Chem. (1964), 76(20), 860

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 62:9095

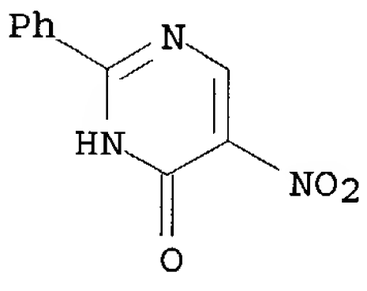
GI For diagram(s), see printed CA Issue.

AB Condensation of MeNO2 with HC(OEt)2-NMe2 (I) 5 hrs. at 60° afforded Me2NCH:CHNO2, which added to PhCONCO over 12 hrs. at 20° to give Me2NCH:C(NO2)-CONHCOPh, which in turn reacted with NH2 in HCONMe2 1 hr. at 0° and subsequently 3 hrs. at 140° to give 4-hydroxy-5-nitro-2-phenylpyrimidine (II), m. 278°, in 42% yield calculated on MeNO2. Similarly, condensation of H2NCH:C(NO2)CONH2 with I at 50° in EtOH gave 4-hydroxy-5-nitropyrimidine, m. 192°, in 20% yield.

IT **3749-46-0**, 4-Pyrimidinol, 5-nitro-2-phenyl-
(preparation of)

RN 3749-46-0 CAPLUS

CN 4(1H)-Pyrimidinone, 5-nitro-2-phenyl- (9CI) (CA INDEX NAME)




L10 ANSWER 65 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1964:45728 CAPLUS

DOCUMENT NUMBER: 60:45728

ORIGINAL REFERENCE NO.: 60:8031c-e

TITLE: Formation of 6-hydroxypteridines by condensation of

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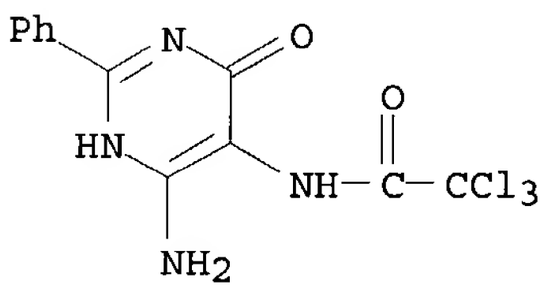
4,5-diaminopyrimidines with chloral
AUTHOR(S): Bergmann, F.; Tamari, M.; Ungar-Waron, Hanna
CORPORATE SOURCE: Hebrew Univ., Jerusalem
SOURCE: Journal of the Chemical Society, Abstracts (1964), (Feb.), 565-72
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Chloral hydrate reacts with 4,5-diaminopyrimidines, bearing O at position 6, to yield 6-hydroxypteridines (I). The ready elimination of all 3 Cl atoms in this condensation contrasts sharply with the resistance of the corresponding 5-di- and 5-trichloroacetamido derivs. to cyclization. It is assumed that the aldehyde group of chloral condenses first with the 5-amino group, the latter then inducing formation of an aziridine ring. This ring opens with simultaneous chloride shift, to produce the chloroimido structure, N: CClCHClOH, in which the hemiacetal group readily condenses with the 4-amino group of the pyrimidine.
IT **91492-97-6**, 4-Pyrimidinol, 6-amino-2-phenyl-5-(2,2,2-trichloroacetamido)-
(preparation of)
RN 91492-97-6 CAPLUS
CN 4-Pyrimidinol, 6-amino-2-phenyl-5-(2,2,2-trichloroacetamido)- (7CI) (CA INDEX NAME)




L10 ANSWER 66 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1964:45727 CAPLUS
DOCUMENT NUMBER: 60:45727
ORIGINAL REFERENCE NO.: 60:8031b-c
TITLE: Reactions of nucleic acids and their components. III. Interaction of adenine and uracil with formaldehyde
AUTHOR(S): Lewin, S.
CORPORATE SOURCE: South-West Essex Tech. Coll., London
SOURCE: Journal of the Chemical Society, Abstracts (1964), (Feb.), 792-809
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. CA 57, 2222f. The interactions of HCHO with adenine (I) and uracil (II) have been examined by using the pH-variation method and spectrophotometry in the temperature range 20-40°. The results with I are interpretable in terms of a major interaction of the unionized N-10 amino group and a minor interaction with the corresponding cation, each with one mol. of HCHO. Evidence for reaction of HCHO with the N-9-H group of purines has been obtained spectrophotometrically. The acid imino group of II also reacts with 1 mol. of HCHO. The reactions of the neutral mols. are exothermic. New structural configurations, involving H-bonded hydrations of the nitrogenous groups of I and II are advocated.
IT **91962-07-1**, 4-Pyrimidinol, 6-amino-5-(2,2-dichloroacetamido)-2-phenyl-
(preparation of)
RN 91962-07-1 CAPLUS

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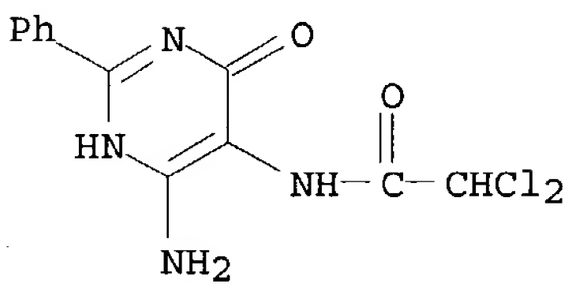
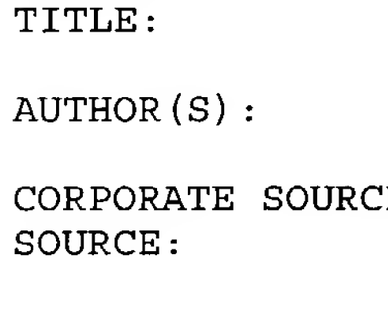
CN 4-Pyrimidinol, 6-amino-5-(2,2-dichloroacetamido)-2-phenyl- (7CI) (CA INDEX NAME)

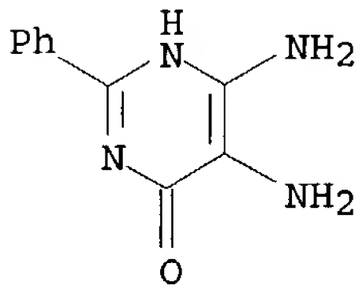


L10 ANSWER 67 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1963:428556 CAPLUS
DOCUMENT NUMBER: 59:28556
ORIGINAL REFERENCE NO.: 59:5168e-g
TITLE: 2-Phenylpurines, their chemical and enzymological reactivity
AUTHOR(S): Bergmann, F.; Kalmus, A.; Ungar-Waron, H.; Kwietny-Govrin, H.
CORPORATE SOURCE: Hebrew Univ.-Hadassah Med. School, Jerusalem
SOURCE: Journal of the Chemical Society, Abstracts (1963) 3729-35
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB 2-Phenylpurines (I) are accessible from 4,5-diamino-2-phenylpyrimidine and its 6-hydroxy and 6- mercapto derivs. Thiation of 2-phenylhypoxanthine proceeds as smoothly as that of hypoxanthine itself. 6,8-Dihydroxy-2-phenylpurine is thiated exclusively at position 6, in contrast to the corresponding 2-methyl derivative Xanthine oxidase is unable to attack position 6 in 2-phenylpurine or its 8-hydroxy derivative, but does so without difficulty in the corresponding 2-methylpurines. 2-Phenylhypoxanthine is oxidized by the enzyme about 50 times faster than the 2-methyl derivative
IT **5466-66-0**, 4-Pyrimidinol, 6-amino-5-nitroso-2-phenyl-
(preparation of)
RN 5466-66-0 CAPLUS
CN 4(1H)-Pyrimidinone, 6-amino-5-nitroso-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 68 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1953:72848 CAPLUS
DOCUMENT NUMBER: 47:72848
ORIGINAL REFERENCE NO.: 47:12395i,12396a-i
TITLE: Investigations of pterins. I. 2-Furyl-4-hydroxypterins
AUTHOR(S): Andrisano, Renato; Maioli, Lillia
CORPORATE SOURCE: Univ. Catania, Italy
SOURCE: Gazzetta Chimica Italiana (1953), 83, 264-8
CODEN: GCITA9; ISSN: 0016-5603
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB In connection with expts. on the pharmacological activity of furyl derivs. (cf. Boll. sci. faculty chim. ind. Bologna 8, 321(1950); C.A. 45, 3851e), some derivs. of the type N:CAr.N:CH.C:C.N:CX.CX':N (I) (where X and X' may be H, OH, Me, Ph, MeC6H4, furyl, or methylfuryl) were prepared in order to establish the influence of the furyl group compared to that of the Ph group. To prepare the pterins, the reaction of Isay [Ber. 39, 250(1906)] was utilized; i.e., the 2-aryl-6-hydroxy-4,5-diaminopyrimidines were condensed with the o-dicarbonyl derivs., with 50-60% yields: N:CAr.N:C(OH).C(NH2):CNH2 (II) + (COX)2 → N:CAr.N:C(OH).C:C.N:CX.CX':N (III). The reactions were carried out in water, dilute AcOH, or concentrated AcOH, by refluxing 0.1 mole II and 0.11 mole diketone for 1-2 hrs. The II compds. were prepared in 3 steps [cf. Boll. accad. gioenia [4] 2, II(1952)]: (1) condensation of ArC(:NH) NH2 compds. with NCCH2CO2Et (IV) to N:CAr. N:C(OH).CH:CNH2 (V) compds. according to the procedure of Maggiolo, et al. (C.A. 46, 2551a); (2) coupling of V with PhN2Cl (VI) to form N:CAr. N:C(OH).C(N: NPh) :CNH2 (VII) compds., and (3) reduction of VII by the method of Benson, et al. (C.A. 44, 10717i) to II. I compds. are soluble in aqueous alkalies and insol. in inorg. acids. They can be well purified by AcOH. NaOMe (0.4 mole in 100 cc. MeOH), 0.1 mole NCCH2CO2Et, and 0.1 mole 2-furylamidine in MeOH, refluxed 2 hrs., distilled in vacuo, the residue taken up in a min. of water, acidified with AcOH, and the precipitate purified by water, yield approx. 58% of 2-furyl-4-amino-6-hydroxypyrimidine (VIII), m. 290°. VI (0.1 mole), added to 0.1 mole VIII in aqueous NaOH (0.2 mole) at 5°, allowed to stand 1 hr., and the precipitate purified by C5H5N, yields almost 100% of 2-furyl-4-amino-5-phenylazo-6-hydroxypyrimidine (IX), yellow, m. 310°. Na2S2O4, added to a suspension of IX in boiling water until the mixture is colorless, allowed to stand, and the precipitate purified by water, yields 92% of 2-furyl-4,5-diamino-6-hydroxypyrimidine (X), m. 231°. Prepared by the procedure used for X, the yield of N:CPh. N:C(OH).CH:CNH2, m. 252°, is 60% (cf. 21% of Baddiley, et al., C.A. 37, 6667.8). Prepared analogously to IX, the yield of 2-phenyl-4-amino-5-phenylazo-6-hydroxypyrimidine, yellow (from C5H5N), m. 306°, is 100%. Prepared analogously to X, the yield of N.CPh. N:C(OH).C(NH2).CNH2, m. 228° (from water), is 80% [cf. Traube and Herrmann, Ber. 37, 2268(1904)]. Eighteen 2-furyl- and 2-phenylpterins of the general constitution III were prepared The following new III are reported [Ar, X, X', empirical formula, color, m.p., time of reaction (min.), reaction solvent, and solvent for purification given]: where Ar = 2-furyl (X = X'): H, C10H6O2N4, light yellow, 288°, 5, water, xylene; HO, C10H6O4N4, light yellow, 330°, 60, water, 30% AcOH; Me, C12H14O2N4, light yellow, 266°, 60, water, xylene; Ph, C22H14O2N4, yellow, 281°, 60, 50% AcOH, AcOH; p-MeC6H4, C24H14O2N4, yellow, 295°, 60, 95% AcOH, AcOH; 2-furyl, C18H10O4N4, yellow, 268°, 60, 50% AcOH, AcOH; 5-methyl-2-furyl, C20H14O4N4, dirty yellow, 220°, 60, 33% AcOH, xylene; Ar = 2-furyl: o,o'-biphenylene, C22H12O2N4, yellow, 373°, 30, 66%, AcOH; 1,2-acenaphthenylene, C20H10O2N4, yellow, 358°, 60, AcOH, AcOH; Ar = Ph (X = X'): H, C12H8ON4, white, 264°, 60, water, xylene; HO, C12H8O3N4, white, 370°, 120, water, water; Me, C14H12ON4, rose, 280°, 60, water, xylene; Ph, C24H16ON4, white, 306°, 60, 7% AcOH, AcOH; p-MeC6H4, C26H20ON4, light yellow, 342°, 60, 95% AcOH, AcOH; 2-furyl, C26H12O3N4, yellow, 322°, 60, 17% AcOH, AcOH; 5-methyl-2-furyl, C22H16O3N4, yellow, 238°, 60, 95% AcOH, EtOH; Ar = Ph: o,o'-biphenylene, C24H14ON4, light yellow, 403-4°, 30, 15% AcOH, C5H5N; 1,2-acenaphthenylene, C22H12ON4, light yellow, 388°, 60, AcOH, AcOH.
IT **61595-45-7**, 4-Pyrimidinol, 5,6-diamino-2-phenyl- (preparation of)
RN 61595-45-7 CAPLUS
CN 4(1H)-Pyrimidinone, 5,6-diamino-2-phenyl- (9CI) (CA INDEX NAME)

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L4             8401 S L1 FUL
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L6              316 S L3 FUL

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L7             1933 S L4 OR L5
L8              878 S L7 NOT (PYRIDYL OR PYRIDIN? OR PYRIMIDIN? OR PYRIMIDYL OR PYR
L9               81 S L8 AND (PHENYL OR NAPHTHYL)
L10              68 S L6
L11              74 S L9 NOT L10

=> d l11 1- ibib abs fhitstr
'L1L' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

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ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
CAN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
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DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
              SCAN must be entered on the same line as the DISPLAY,
              e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, IPC, and NCL

IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
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OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
              containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
              its structure diagram
HITSEQ ------ HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
              its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field
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All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR,
FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC
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ENTER DISPLAY FORMAT (BIB):ibib abs fhitstr
YOU HAVE REQUESTED DATA FROM 74 ANSWERS - CONTINUE? Y/(N):y

L11  ANSWER 1 OF 74  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         2003:870461  CAPLUS
DOCUMENT NUMBER:          139:369336
TITLE:                    Cosmetic compositions containing tetrazoles for
                          increasing hair growth and/or for preventing or hair
                          loss
INVENTOR(S):              Michelet, Jean-Francois; Bernard, Bruno; Rozot, Roger;
                          Boulle, Christophe
PATENT ASSIGNEE(S):       L'Oreal, Fr.
SOURCE:                   Eur. Pat. Appl., 35 pp.
                          CODEN: EPXXDW
DOCUMENT TYPE:            Patent
LANGUAGE:                 French
FAMILY ACC. NUM. COUNT:   2
PATENT INFORMATION:

     PATENT NO.         KIND  DATE           APPLICATION NO.   DATE
     ---------------    ----  --------       ---------------   --------
     EP 1358868          A2   20031105       EP 2003-290990    20030423
     EP 1358868          A3   20031119
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     FR 2838641          A1   20031024       FR 2002-5067      20020423
PRIORITY APPLN. INFO.:                    FR 2002-5067     A   20020423
                                          FR 2002-13461    A   20021028
OTHER SOURCE(S):          MARPAT 139:369336
AB   A cosmetic composition contains an inhibitor of 15-hydroxyprostaglandin
     dehydrogenase and excipient.  The composition can be used to treat hair loss or
     act as a growth stimulant.  Thus, a hair lotion contained 1-phenyl
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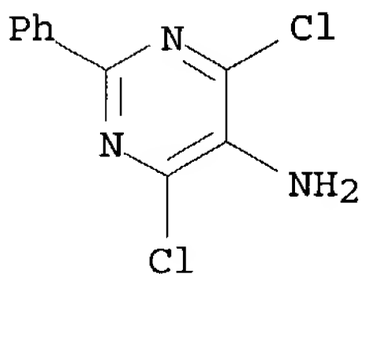
-2-(2-**phenyl**-2H-tetrazol-5-yl)ethanone 0.80, propylene glycol 10.00, and isopropanol qs to 100 g. The composition decreased the hair loss and stimulated hair growth.

IT **20959-02-8**
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(cosmetic compns. containing tetrazoles for increasing hair growth and/or for preventing or hair loss)

RN 20959-02-8 CAPLUS
CN 5-Pyrimidinamine, 4,6-dichloro-2-phenyl- (9CI) (CA INDEX NAME)




L11 ANSWER 2 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:837577 CAPLUS
DOCUMENT NUMBER: 139:341428
TITLE: Hair cosmetic compositions to support the growth and/or delay the fall of hair
INVENTOR(S): Michelet, Jean Francois; Bernard, Bruno
PATENT ASSIGNEE(S): L'Oreal, Fr.
SOURCE: Fr. Demande, 34 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

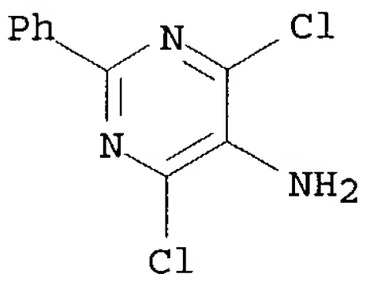
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| FR 2838641 | A1 | 20031024 | FR 2002-5067 | 20020423 |
| EP 1358868 | A2 | 20031105 | EP 2003-290990 | 20030423 |
| EP 1358868 | A3 | 20031119 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| WO 2003090699 | A1 | 20031106 | WO 2003-FR1285 | 20030423 |
| W: CA, JP, US | | | | |

PRIORITY APPLN. INFO.: FR 2002-5067 A 20020423
FR 2002-13461 A 20021028

AB The invention relates to a cosmetic composition containing an inhibitor of the 15-hydroxyprostaglandin dehydrogenase and cosmetic excipients. It also relates to a process of treatment to support the growth and/or to prevent or delay the fall of the hair, as well as the use of an inhibitor of 15-hydroxyprostaglandin dehydrogenase. Thus, 2-**phenyl**-4,6-dichloro-5-aminopyrimidine inhibited the 15-hydroxyprostaglandin dehydrogenase by 43%.

IT **20959-02-8**
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)
(hair cosmetic compns. for delaying fall of hair)

RN 20959-02-8 CAPLUS
CN 5-Pyrimidinamine, 4,6-dichloro-2-phenyl- (9CI) (CA INDEX NAME)

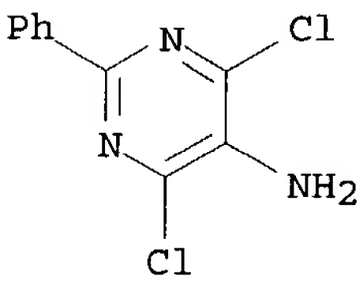


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:804504 CAPLUS
DOCUMENT NUMBER: 140:59596
TITLE: New N6- or N(9)-hydroxyalkyl substituted 8-azaadenines or adenines as effective A1 adenosine receptor ligands
AUTHOR(S): Biagi, Giuliana; Giorgi, Irene; Leonardi, Michele; Livi, Oreste; Pacchini, Federica; Scartoni, Valerio; Costa, Barbara; Lucacchini, Antonio
CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Universita di Pisa, Pisa, I-56126, Italy
SOURCE: European Journal of Medicinal Chemistry (2003), 38(9), 801-810
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In this paper the authors describe synthesis and biol. assays of some A1 ligands more water-soluble than the effective, but very lipophilic, 8-azaadenines and adenines discovered in the past and obtained introducing on N6 or N(9) substituent a hydroxy group. Five of the new N6-hydroxyalkyl- and N6-hydroxycycloalkyl-2-**phenyl**-9-benzyl-8-azaadenines showed very high affinity (Ki<40 nM) and selectivity for A1 adenosine receptors. Among the 2-**phenyl**-9-(2-hydroxy-3-alkyl)-8-azaadenines or adenines prepared, the compds. with the higher A1 affinity and selectivity were 2-**phenyl**-9-(2-hydroxy-3-propyl)-N6-cyclopentyl- and cyclohexyl-8-azaadenine with Ki 2.2±0.2 nM and 2.8±0.3 nM resp. From the point of view of water-solubility, 2-**phenyl**-9-(2-hydroxy-3-propyl)-8-azaadenine was the most interesting compound, having a CLogP of 1.066991 and a water-solubility of 1.2 mg mL-1.

IT **20959-02-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of N6- or N(9)-hydroxyalkyl substituted 8-azaadenines or adenines as effective water-soluble A1 adenosine receptor ligands)
RN 20959-02-8 CAPLUS
CN 5-Pyrimidinamine, 4,6-dichloro-2-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:376819 CAPLUS

09/ 811,359

DOCUMENT NUMBER: 138:385173
TITLE: Preparation of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease
INVENTOR(S): Varghese, John; Maillard, Michel; Jagodzinska, Barbara; Beck, James P.; Gailunas, Andrea; Fang, Larry; Sealy, Jennifer; Tenbrink, Ruth; Freskos, John; Mickelson, John; Samala, Lakshman; Hom, Roy
PATENT ASSIGNEE(S): Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn Company
SOURCE: PCT Int. Appl., 1243 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2003040096 | A2 | 20030515 | WO 2002-US36072 | 20021108 |

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| WO 2003040096 | A2 | 20030515 | WO 2002-XA36072 | 20021108 |

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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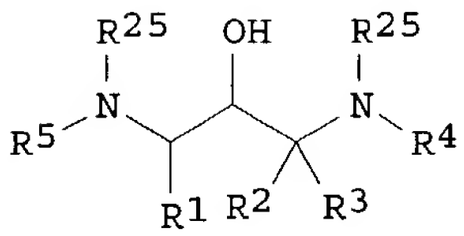
| PRIORITY APPLN. INFO.: | US 2001-337122P | P | 20011108 |
| | US 2001-344086P | P | 20011228 |
| | US 2002-345635P | P | 20020103 |
| | WO 2002-US36072 | A | 20021108 |

OTHER SOURCE(S): MARPAT 138:385173
GI



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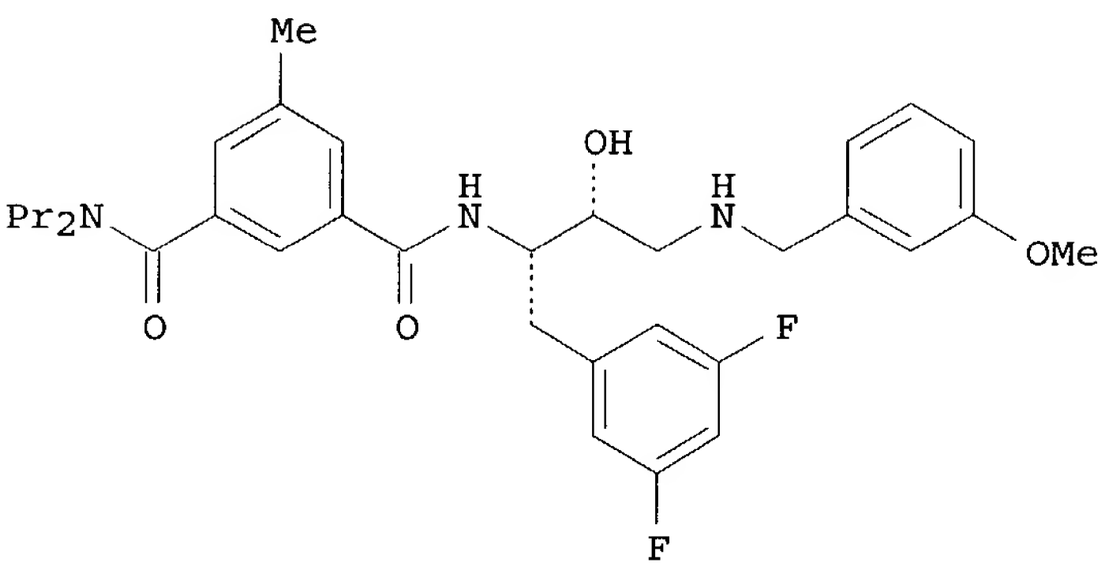


II

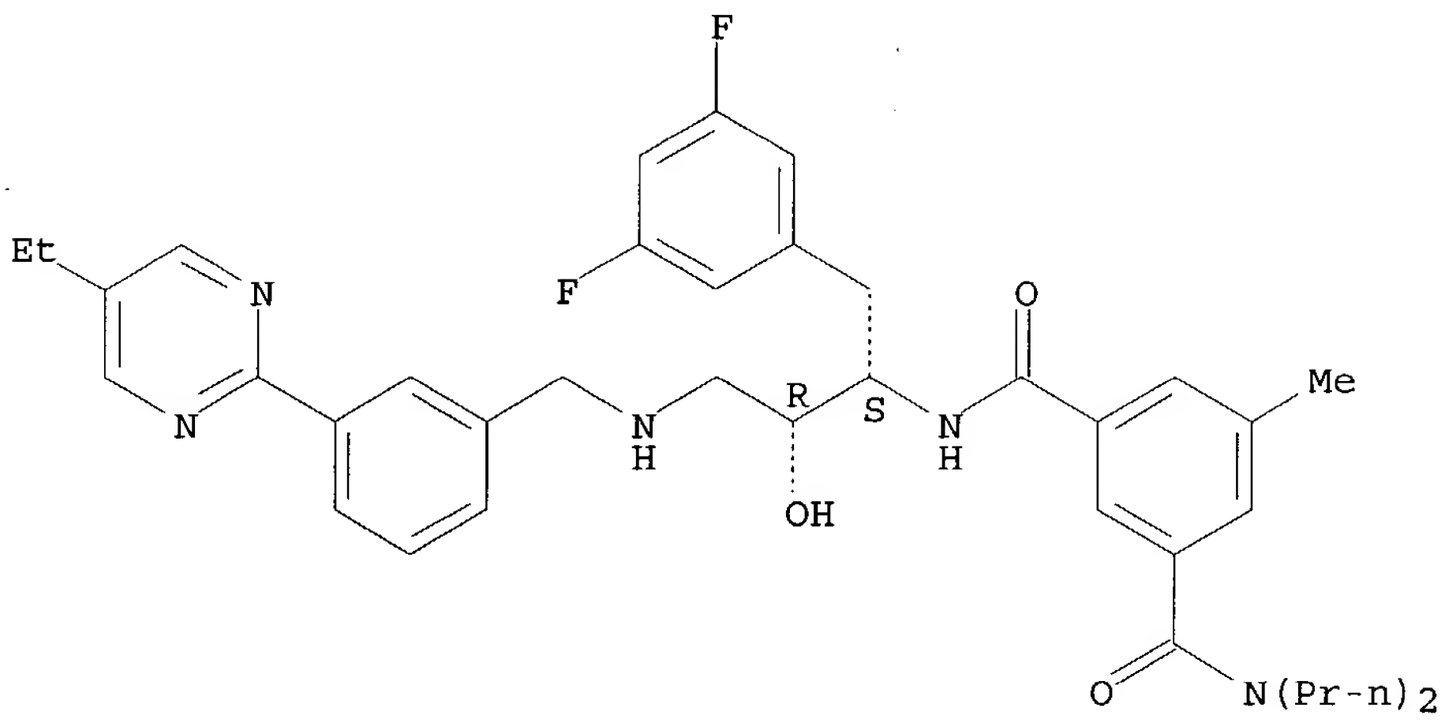
AB The title compds. [I; R1 = (un)substituted alkyl, alkenyl, alkynyl, etc.; R2 = H, alkyl, haloalkyl, alkenyl, etc.; R3 = H, alkyl, haloalkyl, alkenyl, etc.; or R2 and R3 are taken together with the carbon to which they are attached to form a carbocycle of 3-7 carbon atoms, optionally where one carbon atom is replaced by a heteroatom selected from the group consisting of O, S, SO2, (un)substituted NH; R4 = alkyl, haloalkyl, hydroxyalkyl, etc.; R5 = R6X (wherein X = CO, SO2, (un)substituted CH2; R6 = (un)substituted Ph, **naphthyl**, indanyl, etc.); R25 = H, alkyl, alkoxy, etc.] which have activity as inhibitors of β-secretase and are therefore useful in treating a variety of disorders such as Alzheimer's disease, were prepared E.g., a multi-step synthesis of (1S,2R)-II, starting from (2S)-2-[(tert-butoxycarbonyl)amino]-3-(3,5-difluorophenyl)propanoic acid, was given. The compds. I showed IC50 of < 20 μM in cell free inhibition assay utilizing a synthetic APP substrate. This is a Part 1 of 1-2 series.

IT **527729-81-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease)

RN 527729-81-3 CAPLUS

CN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[3-(5-ethyl-2-pyrimidinyl)phenyl]methyl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI) (CA INDEX NAME)

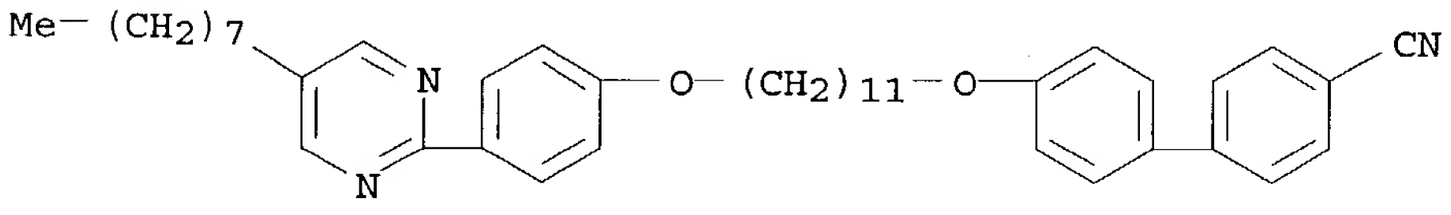
Absolute stereochemistry.




L11 ANSWER 5 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:96444 CAPLUS
DOCUMENT NUMBER: 138:329338
TITLE: A novel frustrated phase produced by a binary system of nonsymmetric dimeric liquid crystals
AUTHOR(S): Yoshizawa, Atsushi; Yamamoto, Kazuyuki; Dewa, Harutada; Nishiyama, Isa; Yamamoto, Jun; Yokoyama, Hiroshi
CORPORATE SOURCE: Department of Materials Science and Technology, Faculty of Science and Technology, Hirosaki University, Hirosaki, 036-8561, Japan
SOURCE: Journal of Materials Chemistry (2003), 13(2), 172-174
CODEN: JMACEP; ISSN: 0959-9428
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A novel frustrated liquid-crystalline phase was obtained in some binary mixts. between polar nonsym. dimeric liquid crystals, α-(4-cyanobiphenyl-4'-yloxy)-ω-[4-(5-alkylpyrimidin-2-yl) **phenyl**-4''-oxy]alkanes; it appeared below nematic or smectic A phases and was found not to possess a clear layered structure.

IT **213549-33-8**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(frustrated phase in binary system of (cyanobiphenylyloxy)[(alkylpyrimidinyl)phenyloxy]alkane liquid crystals)
RN 213549-33-8 CAPLUS
CN [1,1'-Biphenyl]-4-carbonitrile, 4'-[[11-[4-(5-octyl-2-pyrimidinyl)phenoxy]undecyl]oxy]- (9CI) (CA INDEX NAME)




REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:790550 CAPLUS

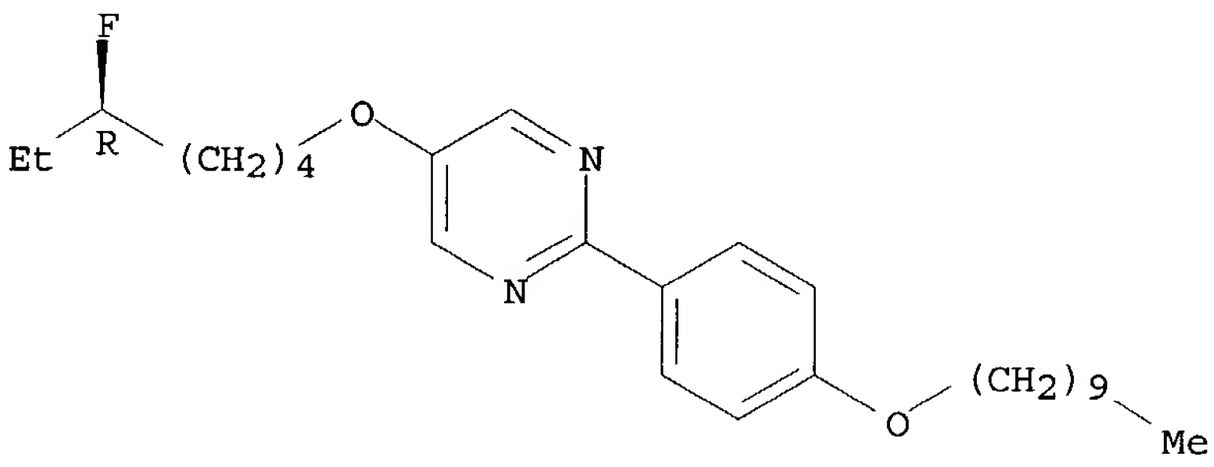
09/ 811,359

DOCUMENT NUMBER: 138:100099
TITLE: Optical resolution of 5-alkyl-δ-valerolactones and synthesis of optically active 5-fluoroalkanols
AUTHOR(S): Riswoko, Asep; Aoki, Yoshio; Hirose, Takuji; Nohira, Hiroyuki
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Saitama University, Urawa, 338-8570, Japan
SOURCE: Enantiomer (2002), 7(1), 33-39
CODEN: EANTE2; ISSN: 1024-2430
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Optical resolns. of 5-alkyl-δ-valerolactones were carried out by derivatization to the diastereomeric amides, in which (R)-(+)-1-(1-**naphthyl**)ethylamine or (S)-(-)-1-phenylethylamine were used as resolving agents. Optically active 5-fluoroalkanols, useful intermediates for fluorinated ferroelec. liquid crystals, were derived from the resolved lactones in four steps without racemization.

IT **483287-73-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and properties of)
RN 483287-73-6 CAPLUS
CN Pyrimidine, 2-[4-(decyloxy)phenyl]-5-[[(5R)-5-fluoroheptyl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

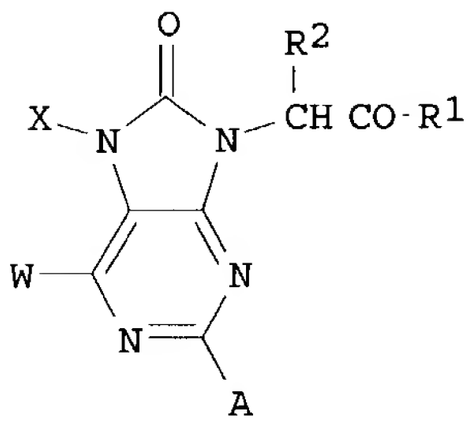



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:439079 CAPLUS
DOCUMENT NUMBER: 137:6192
TITLE: Preparation of 2-(7,8-dihydro-8-oxo-9H-purin-9-yl)acetic acids
INVENTOR(S): Masumoto, Kaoru; Murata, Akiya
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 2002167387 | A2 | 20020611 | JP 2000-362126 | 20001129 |

PRIORITY APPLN. INFO.: JP 2000-362126 20001129
OTHER SOURCE(S): MARPAT 137:6192
GI



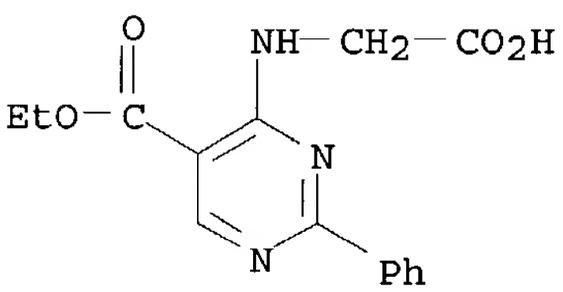
I

AB Title compds. I [R1 = OH, NH2, NHR3; R3 = lower alkyl, alkenyl, cycloalkyl, benzyloxy, etc.; R2 = H, lower alkyl, hydroxyalkyl, (un)substituted benzyloxyalkyl; W = H, lower alkyl, halo, lower alkoxy, NH2, etc.; X = H, lower alkyl, cycloalkylalkyl, phenylalkyl, alkenyl, alkanoyl, etc.; A = (un)substituted Ph, heteroaryl] or their salts are prepared The compds. are useful as materials for anxiety inhibitors, antidepressants, and antiepileptics. 2-(7,8-Dihydro-8-oxo-2-**phenyl**-9H-purin-9-yl)acetonitrile (2.5 g) was treated with NaOH in EtOH at 80° for 2 h to give 1.5 g 2-(7,8-dihydro-8-oxo-2-**phenyl**-9H-purin-9-yl)acetic acid.

IT **226954-91-2**, 2-[(5-Ethoxycarbonyl-2-phenylpyrimidin-4-yl)amino]acetic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (dihydrooxopurinyl)acetic acid)

RN 226954-91-2 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[(carboxymethyl)amino]-2-phenyl-, 5-ethyl ester (9CI) (CA INDEX NAME)



L11 ANSWER 8 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:261297 CAPLUS
DOCUMENT NUMBER: 137:13584
TITLE: Layer compression modulus in smectic liquid crystals
AUTHOR(S): Shibahara, Seiji; Yamamoto, Jun; Takanishi, Yoichi; Ishikawa, Ken; Takezoe, Hideo
CORPORATE SOURCE: Department of Organic and Polymeric Materials, Tokyo Institute of Technology, Tokyo, 152-8552, Japan
SOURCE: Journal of the Physical Society of Japan (2002), 71(3), 802-807
CODEN: JUPSAU; ISSN: 0031-9015
PUBLISHER: Physical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The layer compression modulus B for smectic liquid crystals near the SmA-SmC*, SmA-SmC*A, SmA-ferrielec. phase transitions. B shows a significant pretransitional softening due to the order parameter fluctuations above the phase transitions, suggesting that these phase transitions are not of the Landau mean-field type. B was also measured

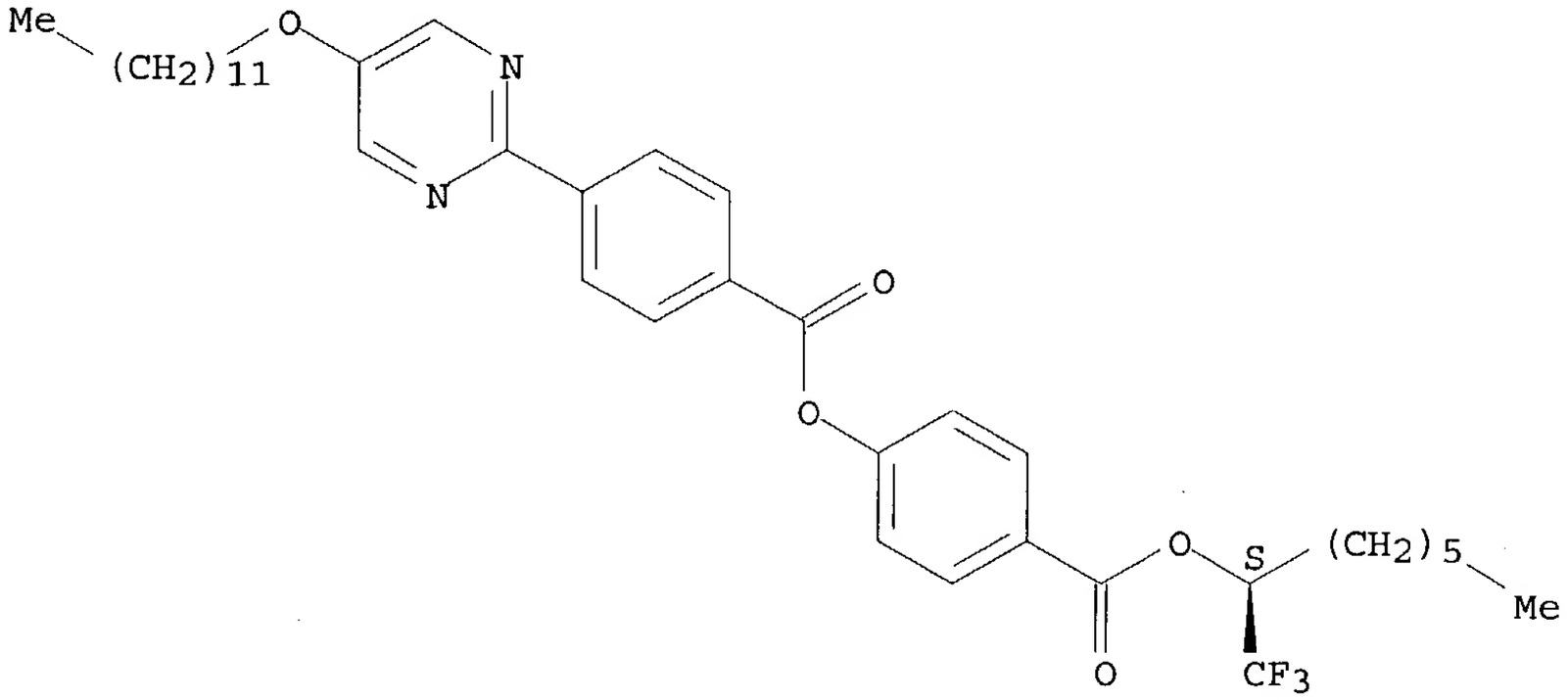
near the nematic-SmA and SmA-CryB phase transitions. In the vicinity of the nematic-SmA phase transition, critical exponent of B is in very good agreement with that determined by light scattering. At the SmA-CryB phase transition, B suddenly increases without pretransitional behavior.

IT **129409-27-4**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(layer compression modulus in smectic liquid crystals near phase transitions)

RN 129409-27-4 CAPLUS

CN Benzoic acid, 4-[5-(dodecyloxy)-2-pyrimidinyl]-, 4-[[[(1S)-1-(trifluoromethyl)heptyl]oxy]carbonyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.




REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

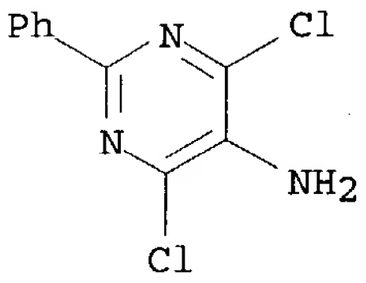
L11 ANSWER 9 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:235346 CAPLUS
DOCUMENT NUMBER: 138:32776
TITLE: erythro- and threo-2-Hydroxynonyl substituted 2-phenyladenines and 2-**phenyl**-8-azaadenines: ligands for A1 adenosine receptors and adenosine deaminase
AUTHOR(S): Biagi, Giuliana; Giorgi, Irene; Livi, Oreste; Pacchini, Federica; Rum, Pietro; Scartoni, Valerio; Costa, Barbara; Mazzoni, Maria Rosa; Giusti, Laura
CORPORATE SOURCE: Department of Pharmaceutical Sciences, University of Pisa, Pisa, 56126, Italy
SOURCE: Farmaco (2002), 57(3), 221-233
CODEN: FRMCE8; ISSN: 0014-827X
PUBLISHER: Editions Scientifiques et Medicales Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Erythro-2-**Phenyl**-9-(2-hydroxy-3-nonyl)adenine and its 8-aza analog were prepared and showed a very high inhibitory activity towards adenosine deaminase (ADA), with Ki 0.55 and 1.67 nM, resp., and high affinity for A1 adenosine receptors, with Ki 28 and 2.8 nM, resp. To increase affinity for A1 receptors we introduced a substituent on the N6 position such as alkyl or cycloalkyl groups, which are present in effective agonists or antagonists. Furthermore, for some compds., we prepared the two diastereoisomers erythro and threo to verify whether the binding with A1 receptors is stereoselective, as in ADA. Results show that some of the synthesized compds. are good inhibitors for ADA and good

ligands for A1, and the erythro diastereoisomers are more active than the threo ones. The exptl. evidence allows us to hypothesize some similarity in the three dimensional structures of the binding site of the two proteins, ADA and A1 adenosine receptor, in spite of lacking any homologies in the amino acid sequences.

IT **20959-02-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(phenyladenines and phenylazaadenines as ligands for A1 adenosine receptors and adenosine deaminase inhibitors)

RN 20959-02-8 CAPLUS
CN 5-Pyrimidinamine, 4,6-dichloro-2-phenyl- (9CI) (CA INDEX NAME)




REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

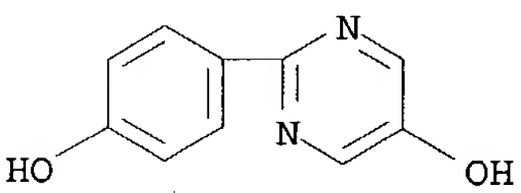
L11 ANSWER 10 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:177700 CAPLUS
DOCUMENT NUMBER: 136:195461
TITLE: Structure-activity relationships for gene activation oestrogenicity: evaluation of a diverse set of aromatic chemicals
AUTHOR(S): Schultz, T. Wayne; Sinks, Glendon D.; Cronin, Mark T. D.
CORPORATE SOURCE: Department of Comparative Medicine, College of Veterinary Medicine, The University of Tennessee, Knoxville, TN, 37996-4500, USA
SOURCE: Environmental Toxicology (2002), 17(1), 14-23
CODEN: ETOXFH; ISSN: 1520-4081
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Structure-activity relationships for estrogenicity were developed based on 120 aromatic chems. evaluated in the Saccharomyces cerevisiae-based Lac-Z reporter assay. Relative gene activation was compared to 17β-estradiol and varied over eight orders of magnitude. Anal. of the data compared to 17β-estradiol identified three structural criteria that were related to xenoestrogen activity and potency: (1) the hydrogen-bonding ability of the phenolic ring mimicking the A-ring, (2) a hydrophobic center similar in size and shape to the B- and C-rings, and (3) a hydrogen-bond donor mimicking the 17β-hydroxyl moiety of the D-ring, especially with an oxygen-to-oxygen distance similar to that between the 3- and 17β-hydroxyl groups of 17β-estradiol. Binding data were segregated into activity clusters including strong, moderate, weak, and detectable gene expression, and those compds. that were inactive. The hydrogen-bonding ability of hydroxy group in the 3-position on 17β-estradiol was observed to be essential for gene activation. Compds. with a 4-hydroxyl substituted benzene ring and a hydrophobic moiety of size and shape equivalent to the B-ring of 17β-estradiol were generally observed to be weakly active compds. Moderately active compds. have a 4-hydroxyl substituted benzene ring with a hydrophobic moiety equivalent in size and shape to the B- and C-ring of 17β-estradiol, or have a high hydrogen-bond donor capacity owing to the presence of halogens on a nonphenolic ring. Strongly active compds., similar to 4,4'-diethylethylene bisphenol (DES), possess the same hydrophobic ring

structure as described for moderately active compds. and an addnl. hydroxyl group with an oxygen-to-oxygen distance close to that exhibited by the 3- and 17-hydroxyl groups of 17β-estradiol.

IT **142172-97-2**
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(structure-activity relationships of diverse set of aromatic chems. for gene activation estrogenicity)

RN 142172-97-2 CAPLUS
CN 5-Pyrimidinol, 2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)




REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 11 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:767018 CAPLUS
Correction of: 1996:672852
DOCUMENT NUMBER: 135:273074
Correction of: 126:31466
TITLE: Boronic acid and ester inhibitors of thrombin
INVENTOR(S): Amparo, Eugene C.; Miller, William H.; Pacofsky, Gregory J.; Wityak, John; Weber, Patricia C.; Duncia, John J. V.; Santella, Joseph B., III
PATENT ASSIGNEE(S): The DuPont Merck Pharmaceutical Company, USA
SOURCE: U.S., 170 pp., Cont.-in-part of U.S. Ser. No. 348,029.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 5563127 | A | 19961008 | US 1994-364338 | 19941227 |
| CA 2208971 | AA | 19960711 | CA 1995-2208971 | 19951213 |
| CA 2208971 | C | 20010116 | | |
| WO 9620689 | A2 | 19960711 | WO 1995-US16248 | 19951213 |
| WO 9620689 | A3 | 19961024 | | |
| W: AU, CA, JP, MX, NZ | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| AU 9646404 | A1 | 19960724 | AU 1996-46404 | 19951213 |
| EP 810858 | A2 | 19971210 | EP 1995-944331 | 19951213 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE | | | | |
| ZA 9510978 | A | 19970627 | ZA 1995-10978 | 19951227 |
| US 5698538 | A | 19971216 | US 1996-690220 | 19960726 |

PRIORITY APPLN. INFO.:
US 1993-36377 B2 19930324
US 1994-318029 B2 19941004
US 1994-348029 A2 19941201
US 1994-364338 A 19941227
WO 1995-US16248 W 19951213

AB Novel boronic acid and ester and carboxyl-modified amino acid compds. R1-Z-CHR2-A (A = organoboryl, BY1Y2; Y1, Y2 = independently OH, F, organoamino, C1-8 alkoxy, Y1Y2 = cyclic boron ester, amide containing N, S, O; etc.; Z = (CH2)mCX, X = amido, thioamido, etc., substituted C1-12 alkyl, alkenyl, etc.; R1 = arylalkenyl, aryl = substituted Ph, **naphthyl**, biphenyl, etc.; R2 = substituted C1-12 alkyl, alkenyl, etc.), which are

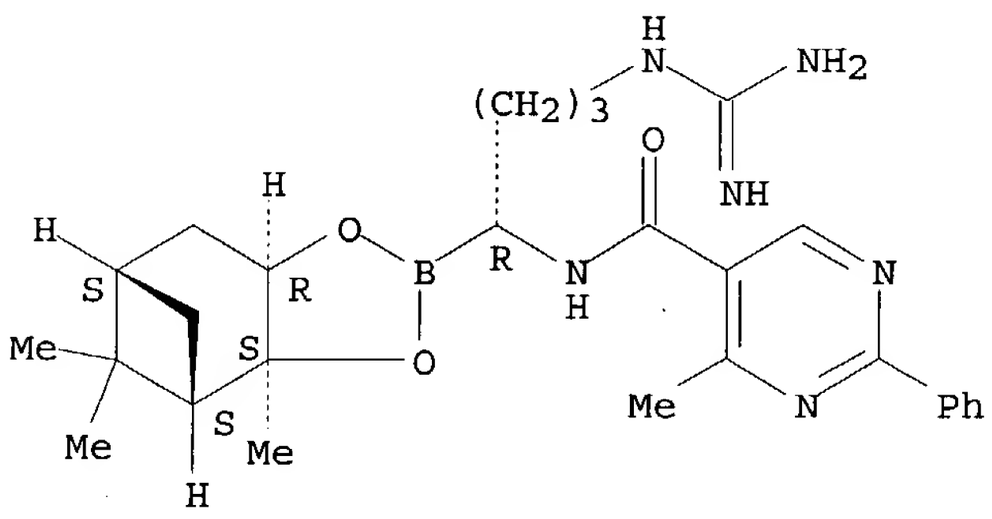
inhibitors of trypsin-like enzymes, are disclosed. Thus, amino acid modified boronic ester (Y1Y2 = (+)-pinanediol) was prepared in multiple steps starting from (+)-pinanediol 4-bromo-1(R)-(4-phenylbenzoyl)aminobutane-1-boronate. Thrombin inhibition activity of some of the compds. prepared is described.

IT **180896-93-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amino acid-modified boronic acids and esters as inhibitors of thrombin)

RN 180896-93-9 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[(1R)-4-[(aminoiminomethyl)amino]-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]butyl]-4-methyl-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




L11 ANSWER 12 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:372157 CAPLUS

DOCUMENT NUMBER: 134:366894

TITLE: Preparation of 2-(4-trifluoromethylphenyl)-4-aminopyrimidines as remedies for autoimmune inflammatory diseases

INVENTOR(S): Murata, Akiya; Kondo, Masanori; Ohno, Kazunori; Tanaka, Masayasu; Ito, Masato

PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

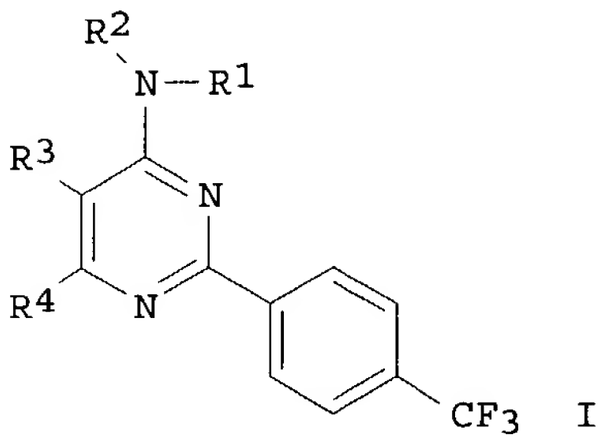
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 2001139560 | A2 | 20010522 | JP 1999-326299 | 19991117 |

PRIORITY APPLN. INFO.: JP 1999-326299 19991117

OTHER SOURCE(S): MARPAT 134:366894

GI



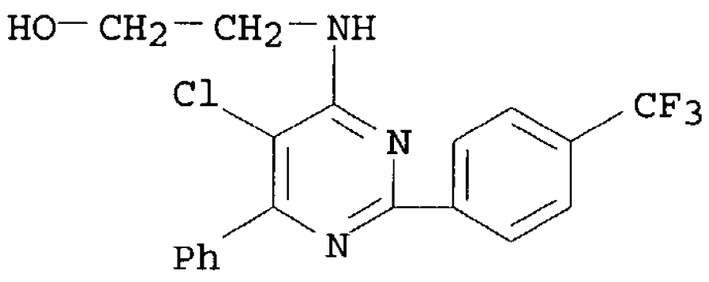
I

AB The title compds. I [R1 = H, alkyl, etc.; R2 = alkyl, etc.; further detail on R1 and R2 is given; R3 = halo, etc.; R4 = alkyl, (un)substituted Ph, etc.] are prepared I [NR1R2 = NHCH2CH(OH)Me; R3 = Cl; R4 = **phenyl** ] at 3 mg/kg/day orally (5 days/wk; for 7.4 wk) gave 98.2 % inhibition of collagen-induced arthritis in mice. Formulations are given.

IT **340149-33-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aminopyrimidines as remedies for autoimmune inflammatory diseases)

RN 340149-33-9 CAPLUS

CN Ethanol, 2-[[5-chloro-6-phenyl-2-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



L11 ANSWER 13 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:238802 CAPLUS

DOCUMENT NUMBER: 135:12839

TITLE: Ferroelectric Liquid Crystals Induced by Atropisomeric Biphenyl Dopants: Dependence of the Polarization Power on the Nature of the Symmetry-Breaking Groups

AUTHOR(S): Vizitiu, Despina; Lazar, Carmen; Radke, Joshua P.; Hartley, C. Scott; Glaser, Matthew A.; Lemieux, Robert P.

CORPORATE SOURCE: Department of Chemistry, Queen's University, Kingston, ON, K7L 3N6, Can.

SOURCE: Chemistry of Materials (2001), 13(5), 1692-1699
CODEN: CMATEX; ISSN: 0897-4756

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

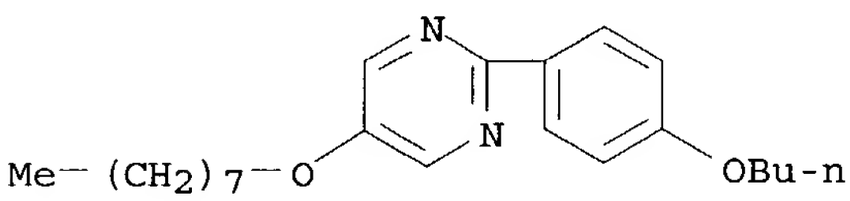
LANGUAGE: English

AB Four new chiral dopants containing an atropisomeric biphenyl core derived from 4,4'-dihydroxy-2,2',6,6'-tetramethylbiphenyl with different symmetry-breaking groups at the 3,3'-positions (X = F, Cl, Br, and Me) were synthesized in optically active form. These dopants were used to induce ferroelec. SmC* liquid crystal phases in four SmC hosts with different core structures. Polarization powers δp were measured as a function of the SmC host and compared to δp values previously obtained for an analogous atropisomeric dopant with X = NO2. Theor.

conformational analyses for rotation of the atropisomeric cores about the C-O bonds of the ester groups linking the core to the side chains were performed at the B3LYP/6-31G(d) level and used in calculating Boltzmann-weighed statistical average transverse dipole moments <μ⊥> for the core-diester units. The <μ⊥> values were used to normalize δp to study the influence of the symmetry-breaking groups X on the polar ordering of the dopants. Variations in δp(norm) are rationalized by considering models describing either achiral or chiral distortions of the zigzag binding site model of the SmC host. The symmetry-breaking groups X exert a unique influence on polar ordering of the dopants in the phenylpyrimidine host PhP1 that is consistent with a model in which chirality transfer via core-core interactions between dopant and host mols. causes a chiral distortion of the zigzag binding site.

IT **121083-89-4**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(ferroelec. Liquid Crystals Induced by Atropisomeric Biphenyl Dopants: Dependence of Polarization Power on Nature of Symmetry-Breaking Groups)

RN 121083-89-4 CAPLUS
CN Pyrimidine, 2-(4-butoxyphenyl)-5-(octyloxy)- (9CI) (CA INDEX NAME)




REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 14 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:235545 CAPLUS
DOCUMENT NUMBER: 134:273626
TITLE: Optically active compound, ferroelectric/antiferroelectric liquid crystal composition, and liquid crystal device using it
INVENTOR(S): Takiguchi, Takao; Hanyu, Yukio; Sato, Koichi; Nakamura, Shinichi; Noguchi, Koji; Shimizu, Yasushi
PATENT ASSIGNEE(S): Canon Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 22 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 2001089421 | A2 | 20010403 | JP 1999-267903 | 19990922 |

PRIORITY APPLN. INFO.: JP 1999-267903 19990922
OTHER SOURCE(S): MARPAT 134:273626

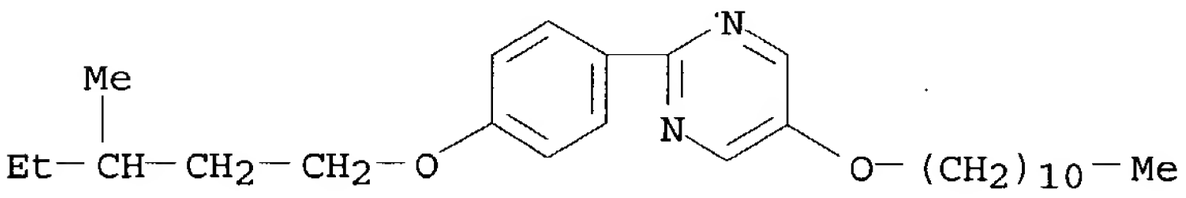
AB The compound comprises RA1X1A2(X2A3)mX3CH(CF3)CH2O(CH2)nB [R = C1-20 alkyl; A1-A3 = (substituted) divalent cyclic group; m = 0, 1; n = 2-20; X1, X2 = none, CO2, O2C, CH2O, OCH2, CH2CH2, CH:CH; C.tplbond.C; X3 = CO2, CH2O, O; B = (substituted) Ph, (substituted) cyclohexyl]. The liquid crystal composition contains the above compound The liquid crystal device comprises the above composition sandwiched between a pair of substrate and a driving electrode. The display shows high response and gives high-contrast images.

IT **108572-55-0D**, mixture containing
RL: DEV (Device component use); USES (Uses)

(optically active compound for ferroelec./antiferroelec. liquid crystal composition used in display)

RN 108572-55-0 CAPLUS

CN Pyrimidine, 2-[4-[(3-methylpentyl)oxy]phenyl]-5-(undecyloxy)- (9CI) (CA INDEX NAME)



L11 ANSWER 15 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:149472 CAPLUS

DOCUMENT NUMBER: 134:340556

TITLE: Ortho-metalated complexes of 2,6-diphenylpyrimidin-4-one

AUTHOR(S): Krylova, L. F.; Terskikh, V. V.

CORPORATE SOURCE: Novosib. Gos. Univ., Russia

SOURCE: Zhurnal Neorganicheskoi Khimii (2000), 45(10), 1714-1720
CODEN: ZNOKAQ; ISSN: 0044-457X

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal

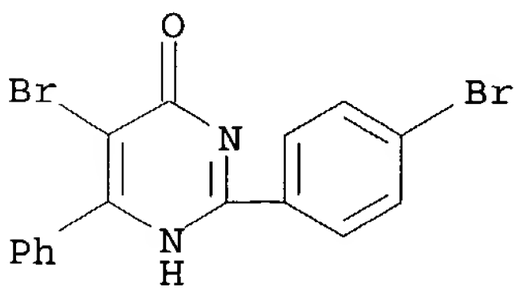
LANGUAGE: Russian

AB Title complexes of Pd(II) and Pt(II) with 2,6-diphenylpyrimidin-4-one (LH2), namely, [Pd(LH)Cl] and [M(L)en] (M = Pt, Pd; en = ethylenediamine), and also the brominated compound 2-(o-bromophenyl)-6-**phenyl**-5-bromopyrimidine-4-one (LBr2) were prepared The o-palladated complex [Pd(LH)Cl] was used as selective reagent. Bromination of [Pd(LH)Cl] under stringent conditions gave LBr2. The structures of the compds. obtained were examined by 1- and 2-dimensional (homo- and heteronuclear) 1H and 13C NMR.

IT **338734-67-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 338734-67-1 CAPLUS

CN 4(1H)-Pyrimidinone, 5-bromo-2-(4-bromophenyl)-6-phenyl- (9CI) (CA INDEX NAME)



L11 ANSWER 16 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:77904 CAPLUS

DOCUMENT NUMBER: 134:280461

TITLE: Gas-phase pyrolysis of 2-heteroaromatic-1-dimethylaminoethylenes: kinetic and mechanistic study

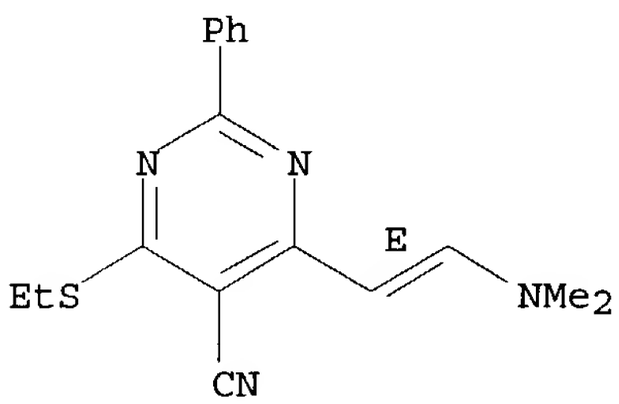
AUTHOR(S): Elnagdi, Mohamed H.; Al-Awadi, Nouria A.; Kumar, Agith; Khalik, Mervat Abdul

CORPORATE SOURCE: Chemistry Department, Kuwait University, Safat, 13060, Kuwait

09/ 811,359

SOURCE: Heteroatom Chemistry (2001), 12(1), 47-51
CODEN: HETCE8; ISSN: 1042-7163
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:280461
AB Gas-phase pyrolysis reactions of 4(2'-dimethylaminoethenyl)-2-oxo-2H-benzo[b]pyran-3-carbonitrile (1), 4(2'-dimethylaminoethenyl)-2-oxo-2H-naphtho[1,2-b]pyran-3-carbonitrile (2), 1,6-dihydro-4-(2'-dimethylaminoethenyl)-6-oxo-1-phenylpyridazine-3,5-dicarbonitrile (3), 2-cyano-5-dimethylamino-3-**phenyl**-2,4-pentadienonitrile (4), 2-cyano-5-dimethylamino-3-(2-thienyl)-2,4-pentadienonitrile (5), 1,2-dihydro-4-(2'-dimethylaminoethenyl)-oxo-quinoline-4-carbonitrile (6), 6-(ethylthio)-4-(2'-dimethylaminoethenyl)-2-phenylpyrimidine-5-carbonitrile (7) have been carried out. The rates of gas-phase pyrolytic reactions of compds. 3, 4, 5, and 7 have been measured and found to correspond to unimol. first-order reactions. Product analyses together with kinetic data were used to outline a feasible pathway for the pyrolytic reactions of the compds. under study.
IT **333722-73-9P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(gas-phase pyrolysis of 2-heteroarom.-1-dimethylaminoethylenes)
RN 333722-73-9 CAPLUS
CN 5-Pyrimidinecarbonitrile, 4-[(1E)-2-(dimethylamino)ethenyl]-6-(ethylthio)-2-phenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.




REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 17 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:441378 CAPLUS
DOCUMENT NUMBER: 133:81642
TITLE: Liquid crystal compound incorporating furan ring for electrooptical display device
INVENTOR(S): Bernhardt, Henry; Kato, Takashi; Fujita, Atsuko; Takeuchi, Hiroyuki; Takeshita, Fusayuki; Nakagawa, Etsuo
PATENT ASSIGNEE(S): Chisso Corporation, Japan
SOURCE: Eur. Pat. Appl., 82 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 1013649 | A1 | 20000628 | EP 1999-125327 | 19991220 |

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

JP 2000191653 A2 20000711 JP 1999-364177 19991222

PRIORITY APPLN. INFO.: US 1998-113506P P 19981222

OTHER SOURCE(S): MARPAT 133:81642

AB The present invention provides a liquid crystal compound incorporating a furan ring having phys. properties suitable for use in an electrooptical display device. The liquid crystal compound may be 5-(4'-trans-pentyl-trans-bicyclohexyl-4-yl)-2-methylfuran, 5-(4-(4-trans-pentylcyclohexyl) **phenyl**)-2-ethylfuran, 5-(trans-4-propylcyclohexyl)fur-2-yl-3,4-dibromobenzene, 2-(4-trans-pentylcyclohexyl)-5-(4-trans-propylcyclohexyl)furan, or 2-(4-trans-(2,3-difluoro-4-methoxyphenyl)cyclohexyl)-5-(5-trans-propyl-1,3-dioxan-2-yl)furan.

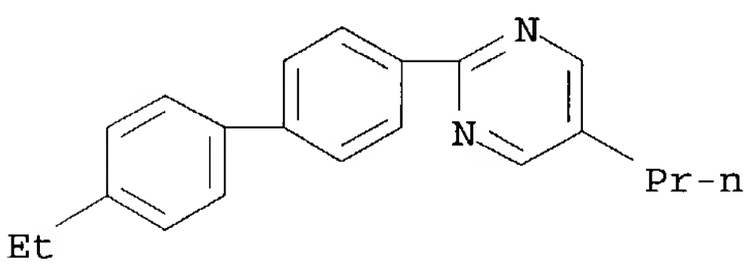
IT **175859-31-1**

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(electrooptical display devices with liquid crystal compns. containing)

RN 175859-31-1 CAPLUS

CN Pyrimidine, 2-(4'-ethyl[1,1'-biphenyl]-4-yl)-5-propyl- (9CI) (CA INDEX NAME)




REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 18 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:335409 CAPLUS

DOCUMENT NUMBER: 132:334474

TITLE: Preparation of spiroindolines as Y5 receptor antagonists

INVENTOR(S): Gao, Ying-duo; Macneil, Douglas J.; Yang, Lihu; Morin, Nancy R.; Fukami, Takehiro; Kanatani, Akio; Fukuroda, Takahiro; Ishii, Yasuyuki; Morin, Masaki

PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Banyu Pharmaceutical Co., Ltd.; et al.

SOURCE: PCT Int. Appl., 130 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000027845 | A1 | 20000518 | WO 1999-US26447 | 19991108 |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 6191160 | B1 | 20010220 | US 1999-436120 | 19991108 |

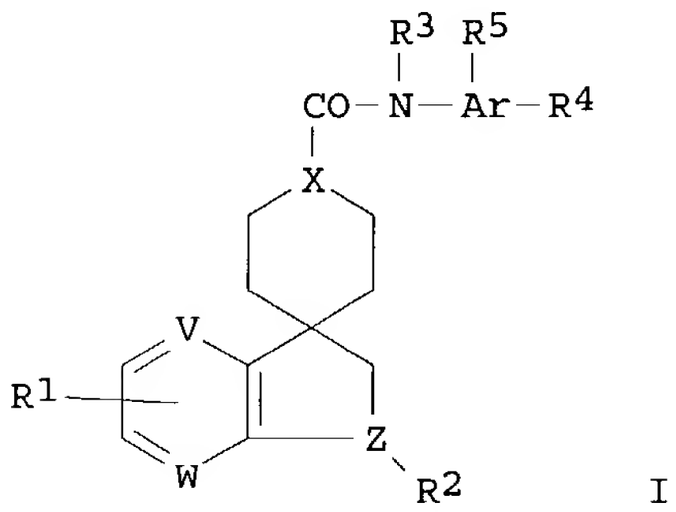
| | | | | |
|---|---|---|---|---|
| EP 1129089 | A1 | 20010905 | EP 1999-971808 | 19991108 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| AU 756797 | B2 | 20030123 | AU 2000-14732 | 19991108 |
| US 6313298 | B1 | 20011106 | US 2000-656698 | 20000907 |
| US 2002058813 | A1 | 20020516 | US 2001-896940 | 20010629 |
| US 6495559 | B2 | 20021217 | | |
| US 6638942 | B1 | 20031028 | US 2002-228250 | 20020826 |

PRIORITY APPLN. INFO.:

| | | | |
|---|---|---|---|
| US 1998-107835P | P | 19981110 |
| US 1999-436120 | A3 | 19991108 |
| WO 1999-US26447 | W | 19991108 |
| US 2000-656698 | A3 | 20000907 |
| US 2001-896940 | A3 | 20010629 |

OTHER SOURCE(S): MARPAT 132:334474


GI



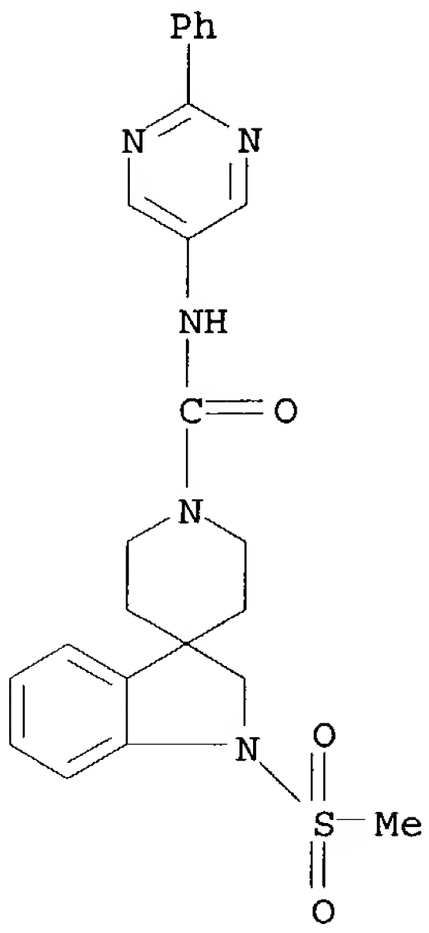
I


AB The title compds. I [V, W, X, Z = CH, N; R1 = H, alkyl, etc.; R2 = CHO, etc.; R3 = H, alkyl; Ar = aryl, heteroaryl; R4, R5 = H, nitro, etc.] are prepared I are useful in the treatment of obesity and the complications associated therewith. 1-Methanesulfonyl-N-(5-**phenyl**-2-pyrazinyl)spiro[indoline-3,4'-piperidine]-1'-carboxamide at 3 mg/kg suppressed bovine pancreatic polypeptide-induced food intake in rats. Formulations are given.


IT **268537-04-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of spiroindolines as Y5 receptor antagonists)

RN 268537-04-8 CAPLUS

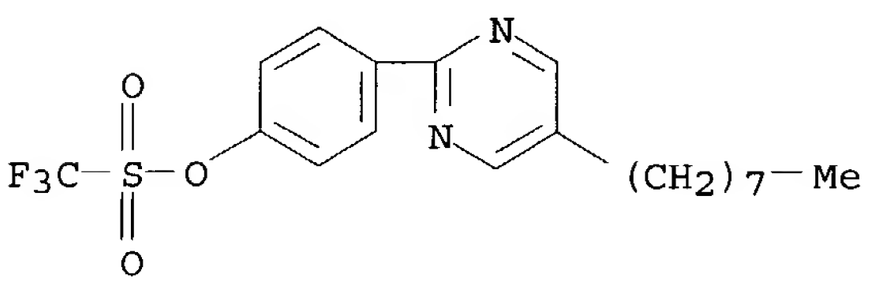
CN Spiro[3H-indole-3,4'-piperidine]-1'-carboxamide, 1,2-dihydro-1-(methylsulfonyl)-N-(2-phenyl-5-pyrimidinyl)- (9CI) (CA INDEX NAME)




REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 19 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:243702 CAPLUS
DOCUMENT NUMBER: 133:17225
TITLE: Nickel- and palladium-catalyzed cross-coupling reactions at the bridgehead of bicyclo[1.1.1]pentane derivatives - a convenient access to liquid crystalline compounds containing bicyclo[1.1.1]pentane moieties
AUTHOR(S): Messner, Matthias; Kozhushkov, Sergei I.; De Meijere, Armin
CORPORATE SOURCE: Institut fur Organische Chemie der George-August-Universitat Gottingen, Gottingen, 37077, Germany
SOURCE: European Journal of Organic Chemistry (2000), (7), 1137-1155
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:17225
AB Radical addition reactions of organyl iodides onto [1.1.1]propellane (I) followed by halogen-lithium exchange and transmetalation with zinc chloride, as well as addns. of Grignard reagents to I, have furnished a variety of 3-substituted bicyclo[1.1.1]pentyl-1-magnesium and -zinc derivs. The latter have been coupled with various alkenyl, aryl, and biaryl halides and triflates under NiCl2dppe, Pd(PPh3)4, or PdCl2(dppf) catalysis to give a number of 1,3-disubstituted bicyclo[1.1.1]pentyl derivs., several of which exhibit liquid crystalline properties, in moderate to very good yields. The coupling products have been further transformed to yield bicyclo[1.1.1]pentyl derivs. bearing alkynyl, cyano, and/or alkenyl groups.
IT **144292-48-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(nickel- and palladium-catalyzed cross-coupling reactions at the bridgehead of bicyclo[1.1.1]pentane derivs.)
RN 144292-48-8 CAPLUS

CN Methanesulfonic acid, trifluoro-, 4-(5-octyl-2-pyrimidinyl)phenyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 82 THERE ARE 82 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 20 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:791837 CAPLUS
DOCUMENT NUMBER: 132:28756
TITLE: Monostable ferroelectric active matrix display
INVENTOR(S): Wingen, Rainer; Nonaka, Toshiaki; Hornung, Barbara
PATENT ASSIGNEE(S): Aventis Research and Technologies GmbH and Co. KG, Germany
SOURCE: Ger. Offen., 18 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 19825484 | A1 | 19991209 | DE 1998-19825484 | 19980608 |
| WO 9964538 | A1 | 19991216 | WO 1999-EP3939 | 19990608 |
| W: BR, CA, CN, CZ, HU, JP, KR, MX, PL, RU, US | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| EP 1086194 | A1 | 20010328 | EP 1999-929151 | 19990608 |
| EP 1086194 | B1 | 20030521 | | |
| R: DE, FR, GB | | | | |
| JP 2002517598 | T2 | 20020618 | JP 2000-553530 | 19990608 |
| US 6551668 | B1 | 20030422 | US 2001-719028 | 20010309 |

PRIORITY APPLN. INFO.: DE 1998-19825484 A 19980608
DE 1998-19830203 A 19980707
WO 1999-EP3939 W 19990608

OTHER SOURCE(S): MARPAT 132:28756

AB The monostable ferroelec. active matrix display contains liquid crystals represented by R1(A1M1)a(A2M2)bA3(M4A4)c(A5M5)dR2 [A3 = fluorinated aromatic ring(s); R1, R2 = H, C2-12-alkyl, alkoxy, etc.; A1, A2, A4, A5 = 1,4-phenylene, 1,3-phenylene, cyclohex-1-en-1,4-diyl, cyclohex-2-en-1,4-diyl, etc.; M1, M2, M3, M5 = single cond, OCO, COO, OCH2, CH2O, CH2CH2, CH2CH2CH2CH2, C.tplbond.C; a, b, c, d = 0, 1], R3(A7M7)a(A8M8)bA6(M9A9)c(A10M10)dR4 [A6 = ring(s); R3, R4 = H, C2-12-alkyl, alkoxy, etc.; A7, A8, A9, A10 = 1,4-phenylene, 1,3-phenylene, cyclohex-1-en-1,4-diyl, cyclohex-2-en-1,4-diyl, etc.; M7, M8, M9, M10 = single cond, OCO, COO, OCH2, CH2O, CH2CH2, CH2CH2CH2CH2, C.tplbond.C; a, b, c, d = 0, 1], R5(A11M11)a(A12M12)bA13 [A13 = substituted **phenyl** ; R5 = H, C2-12-alkyl, alkoxy, etc.; A11, A12 = 1,4-phenylene, 1,3-phenylene, cyclohex-1-en-1,4-diyl, cyclohex-2-en-1,4-diyl, etc.; M11, M12 = single cond, OCO, COO, OCH2, CH2O, CH2CH2, CH2CH2CH2CH2, C.tplbond.C; a, b, c, d = 0, 1], and R6(A14M14)a(A15M15)b(M16A16)c(A17M17)dM18R7 [R6 = H, C2-12-alkyl, alkoxy, etc.; R7 = C3-12-alkyl, etc.; A14-17 = 1,4-phenylene, 1,3-phenylene, cyclohex-1-en-1,4-diyl, cyclohex-2-en-1,4-diyl, etc.; M14-17 = single cond, OCO, COO, OCH2, CH2O,

CH2CH2, CH2CH2CH2CH2, C.tplbond.C; M18 = single cond, OCH2, CH2O, etc.; a, b, c, d = 0, 1].

IT **251934-87-9**
RL: DEV (Device component use); USES (Uses)
(in liquid crystal mixture of monostable ferroelec. active matrix display)

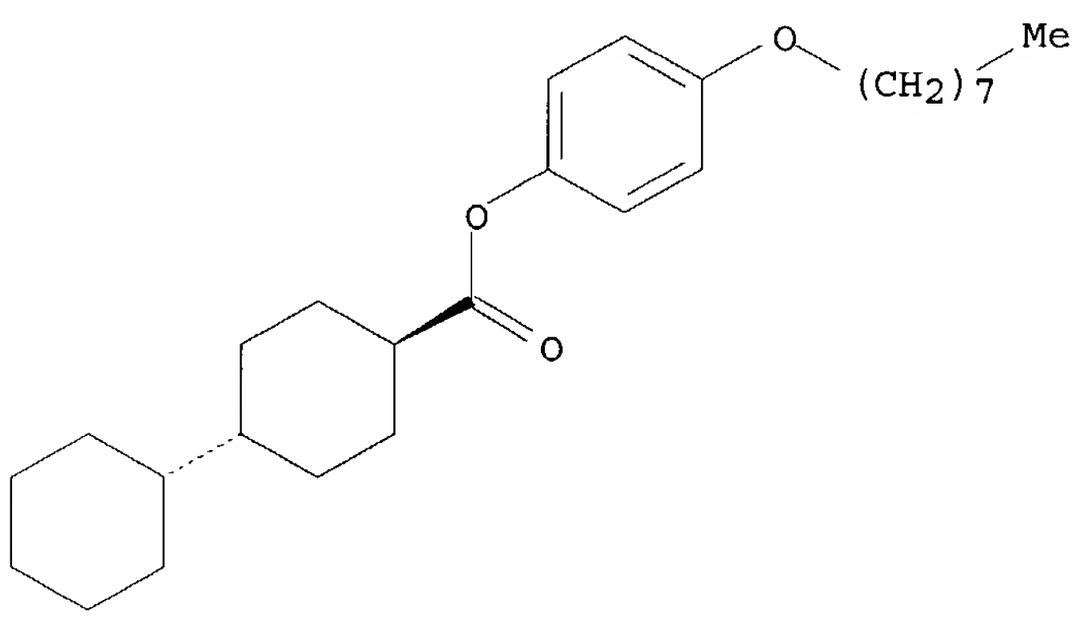
RN 251934-87-9 CAPLUS

CN [1,1'-Bicyclohexyl]-4-carboxylic acid, 4-(octyloxy)phenyl ester, trans-, mixt. with 4-decyl-2,3-difluoro-4''-pentyl-1,1':4',1''-terphenyl, 2,3-difluoro-4-heptyl-4''-pentyl-1,1':4',1''-terphenyl, 2',3'-difluoro-4-(hexyloxy)-4''-pentyl-1,1':4',1''-terphenyl, 2-(4-ethylphenyl)-5-(4-octylphenyl)-1,3,4-thiadiazole, 2'-fluoro-4-(octyloxy)-4''-pentyl-1,1':4',1''-terphenyl, 4-[2-(4-hexylphenyl)-5-thiazolyl]phenyl nonanoate and 5-octyl-2-[4-(octyloxy)phenyl]pyrimidine (9CI) (CA INDEX NAME)

CM 1

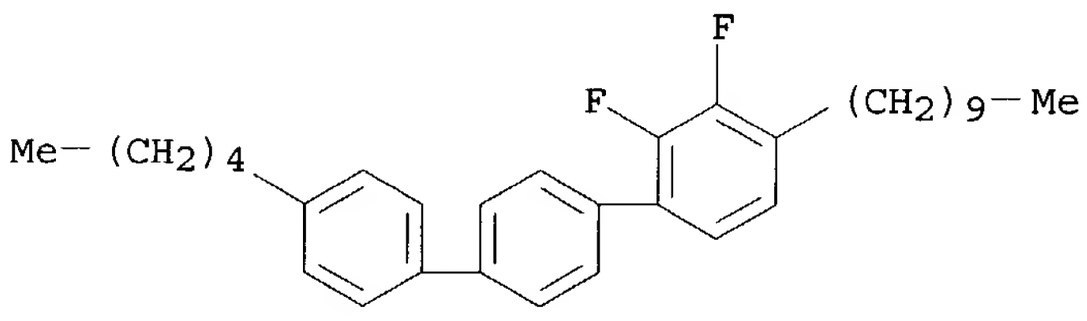
CRN 251934-86-8
CMF C27 H42 O3

Relative stereochemistry.



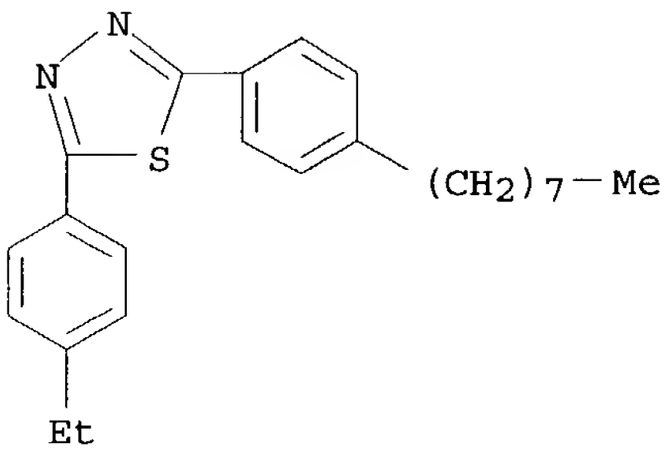

CM 2

CRN 251934-85-7
CMF C33 H42 F2



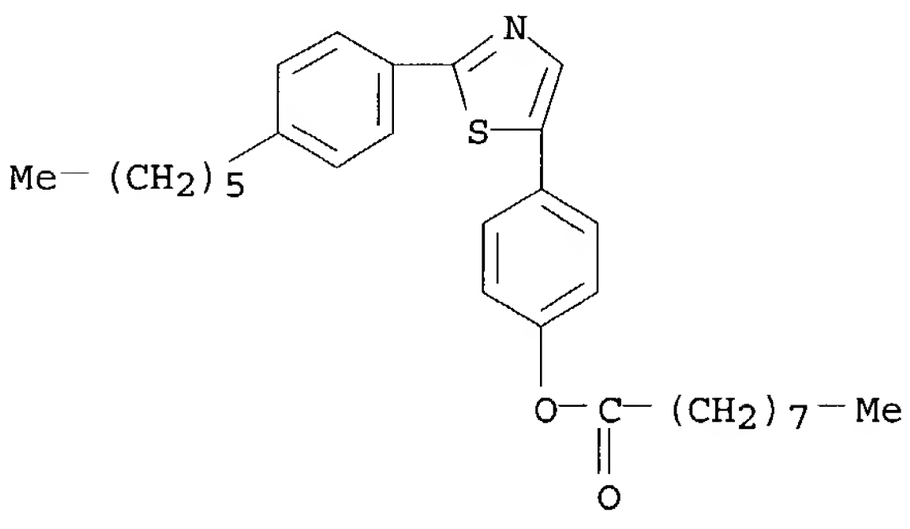

CM 3

CRN 165454-56-8
CMF C24 H30 N2 S



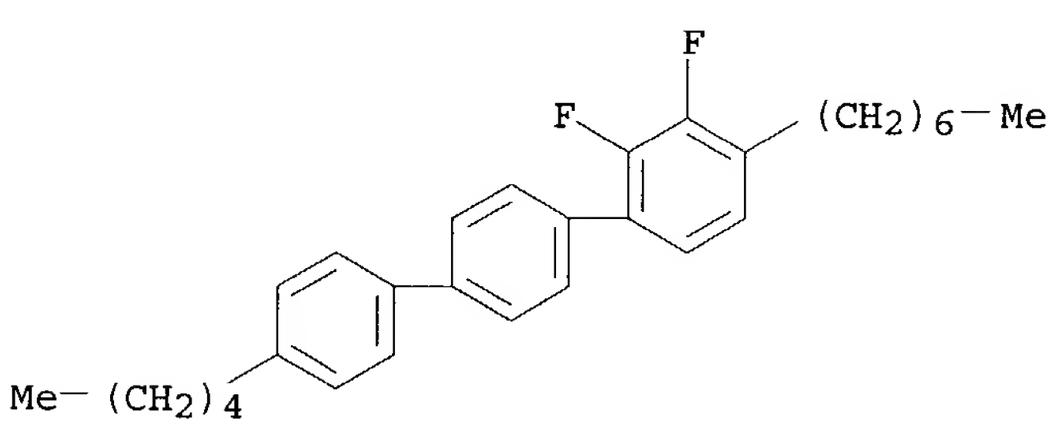
CM 4

CRN 139674-43-4
CMF C30 H39 N O2 S



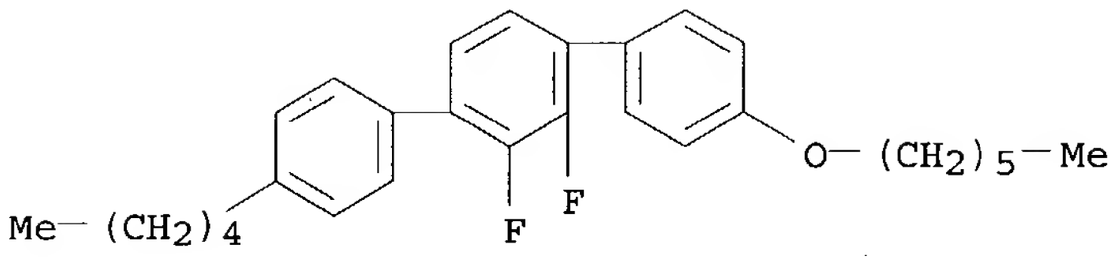
CM 5

CRN 121218-90-4
CMF C30 H36 F2



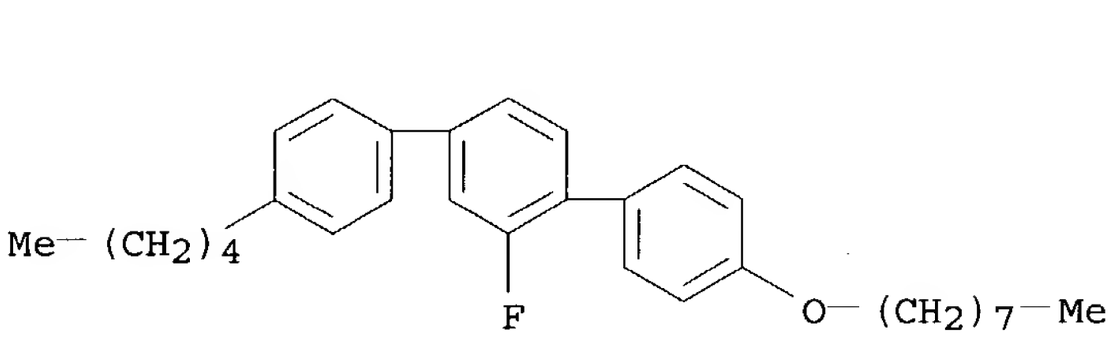
CM 6

CRN 121218-75-5
CMF C29 H34 F2 O



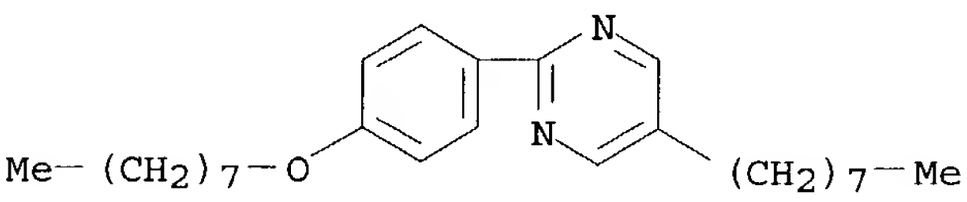
CM 7

CRN 117802-11-6
CMF C31 H39 F O



CM 8

CRN 57202-50-3
CMF C26 H40 N2 O



L11 ANSWER 21 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:661479 CAPLUS
DOCUMENT NUMBER: 132:42727
TITLE: Unified surface anchoring energy for cyano- and fluorinated nematic liquid crystals on a polymer alignment layer
AUTHOR(S): Ishihara, Shoichi; Tsuji, Makoto; Sugimura, Akihiko
CORPORATE SOURCE: LCD Development Group, Display Device Development Center, Matsushita Electric Industrial Co., Ltd., Osaka, 570-8501, Japan
SOURCE: Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1999), 329, 773-782
CODEN: MCLCE9; ISSN: 1058-725X
PUBLISHER: Gordon & Breach Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The unified surface anchoring energy, which is proposed to describe the generalized anisotropic interaction between the nematic director and the substrate, was studied for nematic slabs of various cyano- and fluorinated liquid crystals (LCs) on a polyimide alignment layer. A saturation voltage method, combined with a conventional optical method, was employed for determining the unified surface anchoring energy. The surface anchoring strength (SAS) was found to vary over the range 10-4 to 10-3[J/m2]

depending on the LC mol. structure. It was also found that the values of SAS change with respect to the tilt angle in opposite directions for the cyano- and fluorinated LCs.

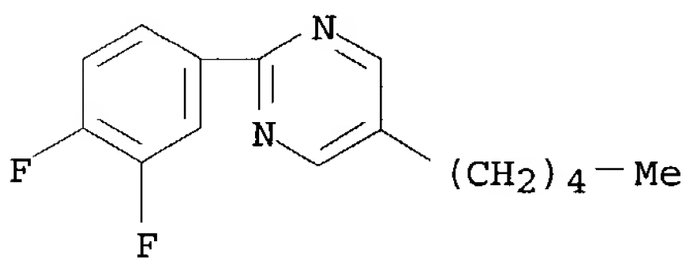
IT **252328-57-7**
RL: PRP (Properties)
(surface anchoring strength on polyimide alignment layer)

RN 252328-57-7 CAPLUS

CN Pyrimidine, 5-butyl-2-(4'-fluoro[1,1'-biphenyl]-4-yl)-, mixt. with 2-(3,4-difluorophenyl)-5-pentylpyrimidine, 2-(3,4-difluorophenyl)-5-propylpyrimidine and 2-(4'-fluoro[1,1'-biphenyl]-4-yl)-5-pentylpyrimidine (9CI) (CA INDEX NAME)

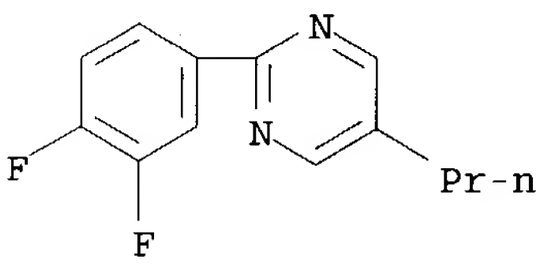
CM 1

CRN 107392-37-0
CMF C15 H16 F2 N2



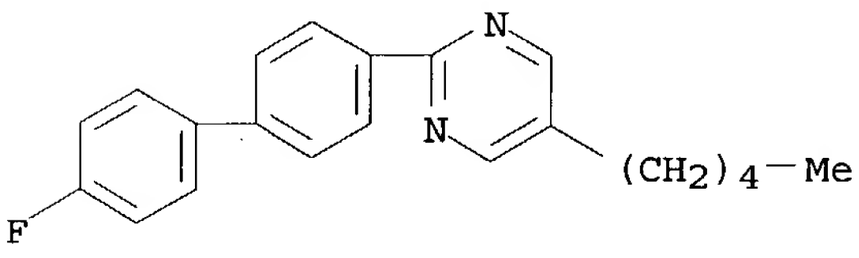

CM 2

CRN 107392-35-8
CMF C13 H12 F2 N2



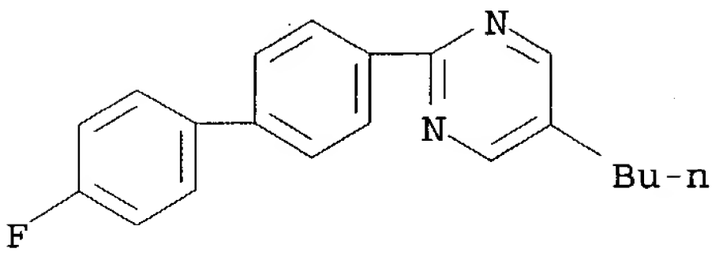

CM 3

CRN 95495-18-4
CMF C21 H21 F N2




CM 4

CRN 95495-17-3
CMF C20 H19 F N2



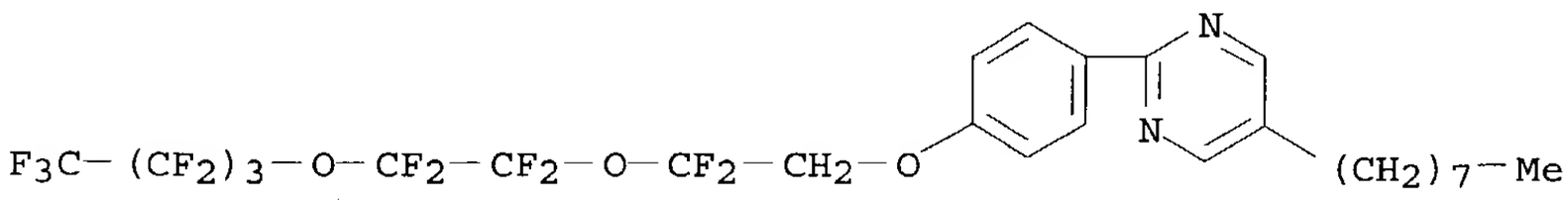

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 22 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:661467 CAPLUS
DOCUMENT NUMBER: 132:7733
TITLE: Smectic layering at the free surface of isotropic liquid crystals in the pre-smectic temperature region characterized by ellipsometry
AUTHOR(S): Glorieux, Christ; De Schrijver, Peter; Johnson, Patrick M.; Balus, Oana; Serban, Constantin; Huang, Cheng Cher; Thoen, Jan
CORPORATE SOURCE: Laboratorium voor Akoestiek en Thermische Fysica, Departement Natuurkunde, K.U. Leuven, Louvain, B-3001, Belg.
SOURCE: Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1999), 329, 663-670
CODEN: MCLCE9; ISSN: 1058-725X
PUBLISHER: Gordon & Breach Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The angular dependence of the ellipsometric signal of bulk isotropic dodecylcyanobiphenyl (12CB) as a function of temperature in the pre-smectic temperature region was determined Using a simple model, the order parameter of the discontinuously growing smectic surface layer was determined approaching the isotropic-smectic phase transition temperature Also the pretransitional isotropic region of the isotropic-smectic transition of the liquid crystal compound 2-(4-(1,1-dihydro-2-(2-perfluorobutoxy)perfluoroethoxy)perfluoroeth oxy)**phenyl**-5-octylpyrimidine (H8F(4,2,1)MOPP) was studied.

IT **152914-98-2**, 2-(4-(1,1-Dihydro-2-(2-perfluorobutoxy)perfluoroethox y)perfluoroethoxy)**phenyl**-5-octylpyrimidine
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(smectic layering at free surface of isotropic liquid crystals in pre-smectic temperature region characterized by ellipsometry)

RN 152914-98-2 CAPLUS
CN Pyrimidine, 2-[4-[2,2-difluoro-2-[1,1,2,2-tetrafluoro-2-(nonafluorobutoxy)ethoxy]ethoxy]phenyl]-5-octyl- (9CI) (CA INDEX NAME)




REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 23 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:567096 CAPLUS
DOCUMENT NUMBER: 132:102399
TITLE: Synthesis and antitumor activity of N'-(benzylidene-

and ethylidene)hydrazides of 2-hydroxy- and 2-**phenyl**-6-hydroxy-4-methylpyrimidyl-5-acetic acids

AUTHOR(S): Khachatryan, V. E.; Israelyan, S. G.; Stepanyan, G. M.; Arsenyan, F. G.; Garibjanyan, B. T.; Melik-Ohanjanyan, R. G.

CORPORATE SOURCE: Inst. Tonkoi Org. Khim. im. A.A. Mndzhoyana, NAN Respubl. Arm., Yerevan, Armenia

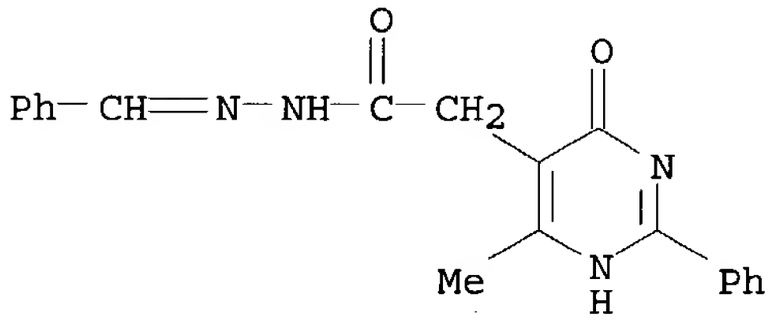
SOURCE: Khimicheskii Zhurnal Armenii (1999), 52(1-2), 102-106
CODEN: KZARF3
PUBLISHER: Izdatel'stvo Gitutyun NAN Respubliki Armenii
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB The series of N'-(benzylidene- and ethylidene)hydrazides of 2-hydroxy- and 2-**phenyl**-6-hydroxy-4-methylpyrimidyl-5-acetic acids were synthesized by the i reaction of appropriate hydrazides with aromatic aldehydes or ketones in ethanol or DMF in the presence of catalytic amts. of concentrated hydrochloric acid. The structure of newly obtained compds. was proved by UR-, NMR- and mass spectroscopy. Toxicity and antitumor activity of these compds. was investigated. The majority of them showed low toxicity and moderate antitumor activity on Sa-45, Sa-37, WCS exptl. tumors. The p-fluorobenzylidene hydrazide of met-acyl-5-acetic acid and p-bromoethylidene hydrazide of 2-**phenyl**-4-hydroxy-6-methylpyrimidyl-5-acetic acid were the most active compds. These substances showed moderate activity on LLC and was non-effective against La hemocytoblastosis.

IT **255867-67-5P**
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and antitumor activity of benzylidene- and ethylidene-hydrazides of hydroxy- and phenylhydroxymethylpyrimidylacetic acids)

RN 255867-67-5 CAPLUS

CN 5-Pyrimidineacetic acid, 1,4-dihydro-6-methyl-4-oxo-2-phenyl-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)




L11 ANSWER 24 OF 74 CAPLUS 

ACCESSION NUMBER: 1999:358691 CAPLUS
DOCUMENT NUMBER: 131:109179

TITLE: Smectic A and C materials with novel director tilt and layer thickness behavior

AUTHOR(S): Radcliffe, Marc D.; Brostrom, Myles L.; Epstein, Kenneth A.; Rappaport, Aaron G.; Thomas, Britt N.; Shao, Renfan; Clark, Noel A.

CORPORATE SOURCE: 3M Company, St. Paul, MN, 55144, USA

SOURCE: Liquid Crystals (1999), 26(6), 789-794
CODEN: LICRE6; ISSN: 0267-8292
PUBLISHER: Taylor & Francis Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

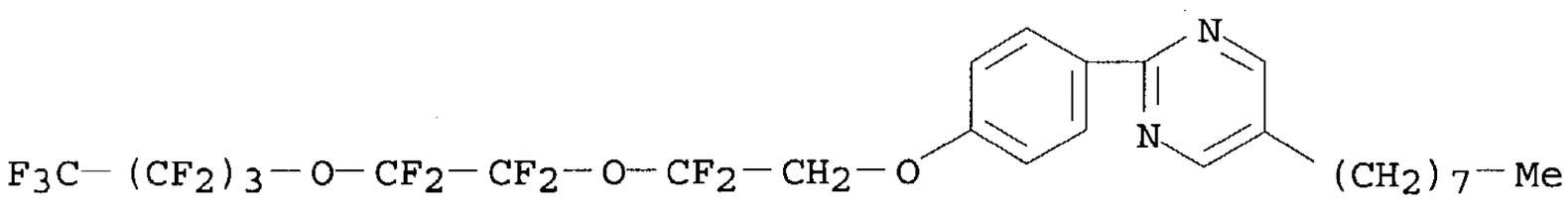
AB The authors report a smectic liquid crystal in which a tilt of the mol.

orientation away from the layer normal in the Smectic C phase of up to 240 occurs with minimal layer contraction. This characteristic, accompanied by an exceptionally large underlying neg. thermal layer expansion coefficient, enables the formation of chiral smectic electrooptical cells having nearly the ideal 'bookshelf' layer geometry, free from the complexities of the chevron layer structure produced by contraction.

IT **152914-98-2**, 2-{4-[1,1-Dihydro-2-(2-perfluorobutoxyperfluoroethoxy)perfluoroethoxy]}**phenyl**-5-octylpyrimidine
RL: PRP (Properties)
(director tilt away from layer normal in relation to layer thickness behavior in smectic C and A liquid crystals in relation to formation of chiral smectic electrooptical cells with bookshelf layer geometry)

RN 152914-98-2 CAPLUS

CN Pyrimidine, 2-[4-[2,2-difluoro-2-[1,1,2,2-tetrafluoro-2-(nonafluorobutoxy)ethoxy]ethoxy]phenyl]-5-octyl- (9CI) (CA INDEX NAME)

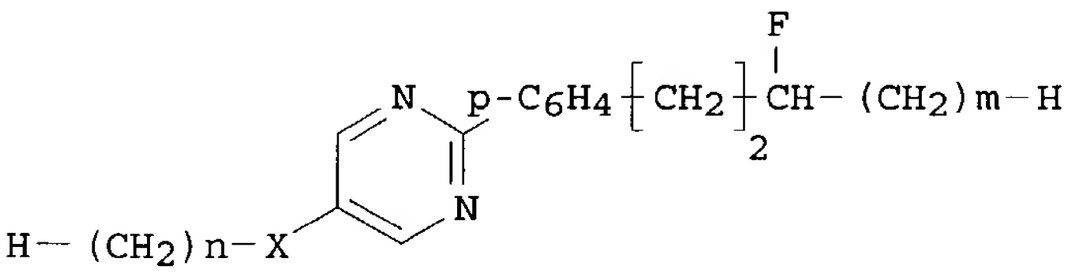


REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 25 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:225668 CAPLUS
DOCUMENT NUMBER: 130:252374
TITLE: Preparation of optically active 3-fluoroalkylphenylpyrimidines for ferroelectric liquid crystals
INVENTOR(S): Kusumoto, Tetsuo; Kato, Miho; Sato, Kenichi; Hiyama, Tamejiro
PATENT ASSIGNEE(S): Sagami Chemical Research Center, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 11092457 | A2 | 19990406 | JP 1997-259515 | 19970925 |

PRIORITY APPLN. INFO.: JP 1997-259515 19970925
OTHER SOURCE(S): CASREACT 130:252374; MARPAT 130:252374
GI



I

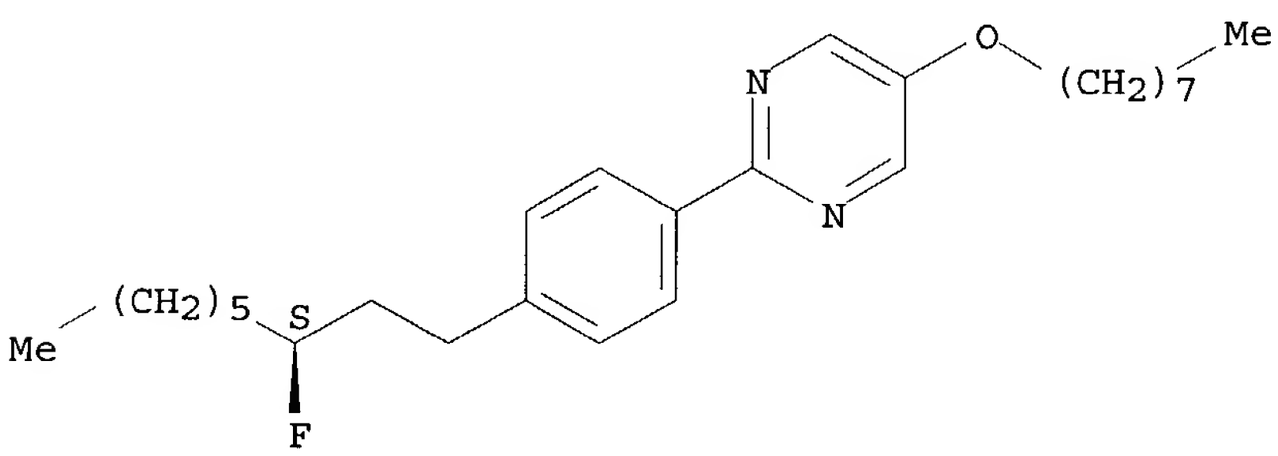
AB Title compds. I (m = 1-16; n = 1-20; X = single bond, O), useful as ferroelec. liquid crystal materials (no data), are prepared by reaction of 4-methylbenzonitrile with optically active Q(CH2)mH (Q = oxiranyl; m =

1-16) in the presence of bases, fluorination of optically active p-NCC6H4CH2CH2CH(OH)(CH2)mH (m = 1-16), reaction of optically active p-NCC6H4CH2CH2CHF(CH2)mH (m = 1-16) with hydrogen halides and alcs., reaction with NH3, reaction with H(CH2)nXC(CHO):CHNMe2 (n, X = same as I). 4-Methylbenzonitrile was reacted with (R)-1,2-epoxyoctane in the presence of (i-Pr)2NH and BuLi in THF at room temperature for 2 h and fluorinated with Et2NSF3 in CH2Cl2 at room temperature to give (S)-4-(3-fluorononyl)benzonitrile, which was reacted with HCl and EtOH in CH2Cl2-ether at room temperature for 4 h, reacted with NH3 at room temperature for 5 days, and cyclized with 3-(N,N-dimethylamino)-2-octyloxyacrolein in a NaOMe/MeOH solution under reflux overnight to give 36% (S)-2-[4-(3-fluorononyl)**phenyl**]-5-octyloxypyrimidine.

IT **152291-78-6P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(preparation of optically active fluoroalkylphenylpyrimidines by ring opening of oxiranes with methylbenzonitrile, fluorination, and cyclization)

RN 152291-78-6 CAPLUS
CN Pyrimidine, 2-[4-[(3S)-3-fluorononyl]phenyl]-5-(octyloxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




L11 ANSWER 26 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:121831 CAPLUS
DOCUMENT NUMBER: 130:318814
TITLE: Designing banana-shaped liquid crystals without Schiff's base units: m-terphenyls, 2,6-diphenylpyridines and V-shaped tolane derivatives
AUTHOR(S): Shen, Dong; Diele, Siegmar; Pelzl, Gerhard; Wirth, Ina; Tschierske, Carsten
CORPORATE SOURCE: Institut fur Organische Chemie, Martin-Luther-Universitat Halle-Wittenberg, Halle, D-06120, Germany
SOURCE: Journal of Materials Chemistry (1999), 9(3), 661-672
CODEN: JMACEP; ISSN: 0959-9428
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This paper reports attempts to obtain (anti)ferroelec. switchable achiral banana-shaped mols. without Schiff's base units. For this purpose the authors synthesized novel V-shaped mols. consisting of rigid angular central units [1,3-disubstituted benzene, 2,7-disubstituted naphthalene, 1,3-diphenylbenzene, 2,6-diphenylnitrobenzene, 2,6-diphenylpyridine, 1,3-bis(phenylethynyl)benzene, 1-**phenyl**-3-(phenylethynyl)benzene] connected via ester linkages to two rigid cores (1,4-disubstituted benzenes, biphenyls, 2-phenylpyrimidines, phenylbenzoates). Most compds. have rather high m.ps. Only mols. with seven aromatic rings show liquid crystalline properties. Two-dimensional modulated smectic phases (rectangular columnar phases) were found for mols. with

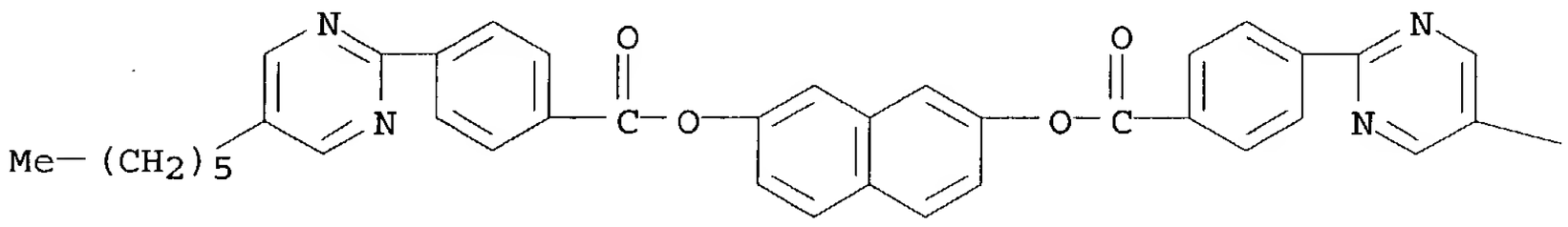
phenylbenzoate rigid units. Intercalated fluid smectic phases were detected for the corresponding 2-phenylpyrimidine derivs. For the 1st time in the case of banana-shaped mols. a nematic phase was observed for a 2'-nitro-m-terphenyl-4,4''-diyl bisbenzoate. However, none of the synthesized compds. exhibit the typical texture of the (anti)ferroelec. switchable mesophases, known from the Schiff's base derivs.

IT **223654-83-9P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation and characterization of)

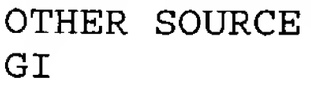
RN 223654-83-9 CAPLUS

CN Benzoic acid, 4-(5-hexyl-2-pyrimidinyl)-, 2,7-naphthalenediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

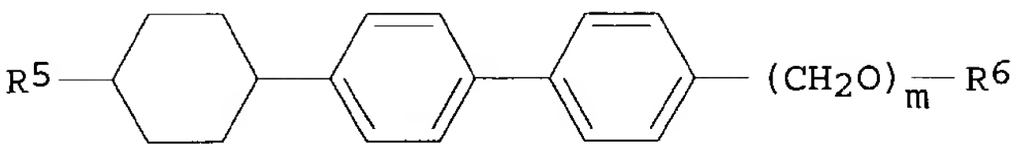


REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

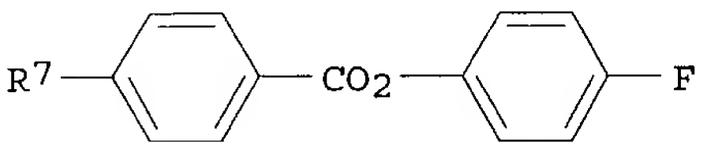
L11 ANSWER 27 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:535947 CAPLUS
DOCUMENT NUMBER: 129:223608
TITLE: Smectic liquid-crystal composition for information recording media
INVENTOR(S): Fukumasa, Mitsumutsu; Okada, Tomomi; Yoshisawa, Atsushi
PATENT ASSIGNEE(S): Japan Energy K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 10219251 | A2 | 19980818 | JP 1997-42890 | 19970213 |

PRIORITY APPLN. INFO.: JP 1997-42890 19970213
OTHER SOURCE(S): MARPAT 129:223608
GI



I



II

AB The media have (A) 4-alkyl-4-cyanobiphenyl and/or 4-alkoxy-4-cyanobiphenyl and (B) R1A1CO2CH2CH(Me)(CH2)nCH(Me)CH2OCOB1R2, R3A2OCOCH(Me)CH2CO2B2R4, I, and/or II (R1-7 = alkyl, alkoxy; A1, B1, A2, B2 = phenylpyrimidine, biphenyl, **phenyl**:benzoic acid, phenylcyclohexane, **phenyl**:biphenylcarboxylic acid, biphenyl:benzoic acid, terphenylpyrimidine, 1,5-diphenylpyrimidine; n = 3-15 integer; m = 0, 1). The composition displays phase transformation by lower voltage application. The composition is useful for high quality and high contrast information recording such as an electrophotog. material, an optical sensor, etc.

IT **212554-10-4**
RL: DEV (Device component use); USES (Uses)
(liquid crystal mixture; nematic liquid crystal mixture containing alkyl or alkoxy cyanobiphenyl for information recording media)

RN 212554-10-4 CAPLUS

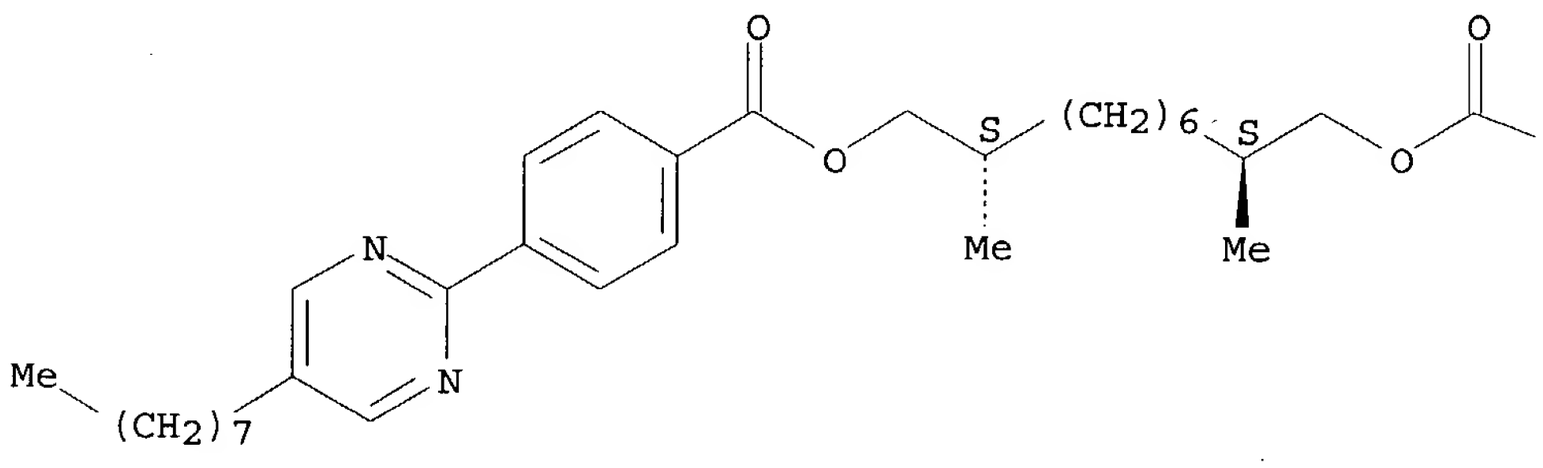
CN Benzoic acid, 4-(5-octyl-2-pyrimidinyl)-, (2S,9S)-2,9-dimethyl-1,10-decanediyl ester, mixt. with 4'-dodecyl[1,1'-biphenyl]-4-carbonitrile, 4'-nonyl[1,1'-biphenyl]-4-carbonitrile and 4'-(nonyloxy)[1,1'-biphenyl]-4-carbonitrile (9CI) (CA INDEX NAME)

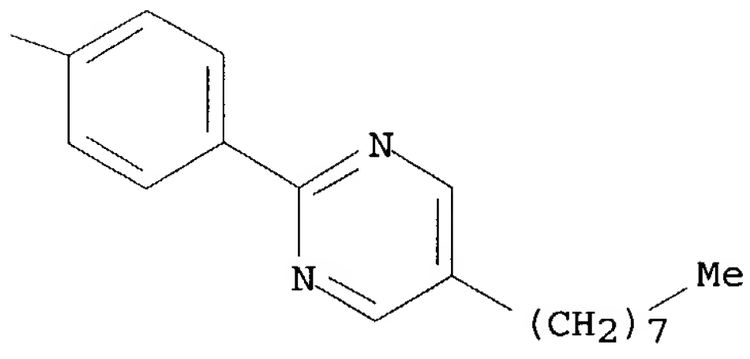
CM 1

CRN 212554-09-1
CMF C50 H70 N4 O4

Absolute stereochemistry.

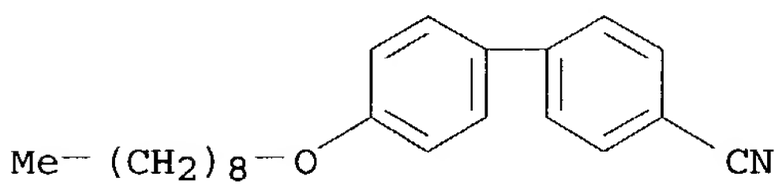






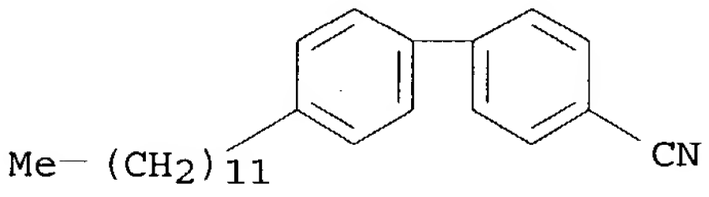
CM 2

CRN 58932-13-1
CMF C22 H27 N O



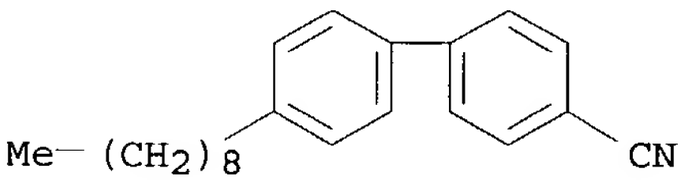
CM 3

CRN 57125-49-2
CMF C25 H33 N



CM 4

CRN 52709-85-0
CMF C22 H27 N



L11 ANSWER 28 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:385479 CAPLUS
DOCUMENT NUMBER: 129:54375
TITLE: Arthropodicidal and fungicidal cyclic amides [triazolones] and their preparation, use, and compositions
INVENTOR(S): Brown, Richard James; Chan, Dominic Ming-Tak; Howard, Michael Henry, Jr.; Daniel, Dilon Jancey; Clark, David

09/ 811,359

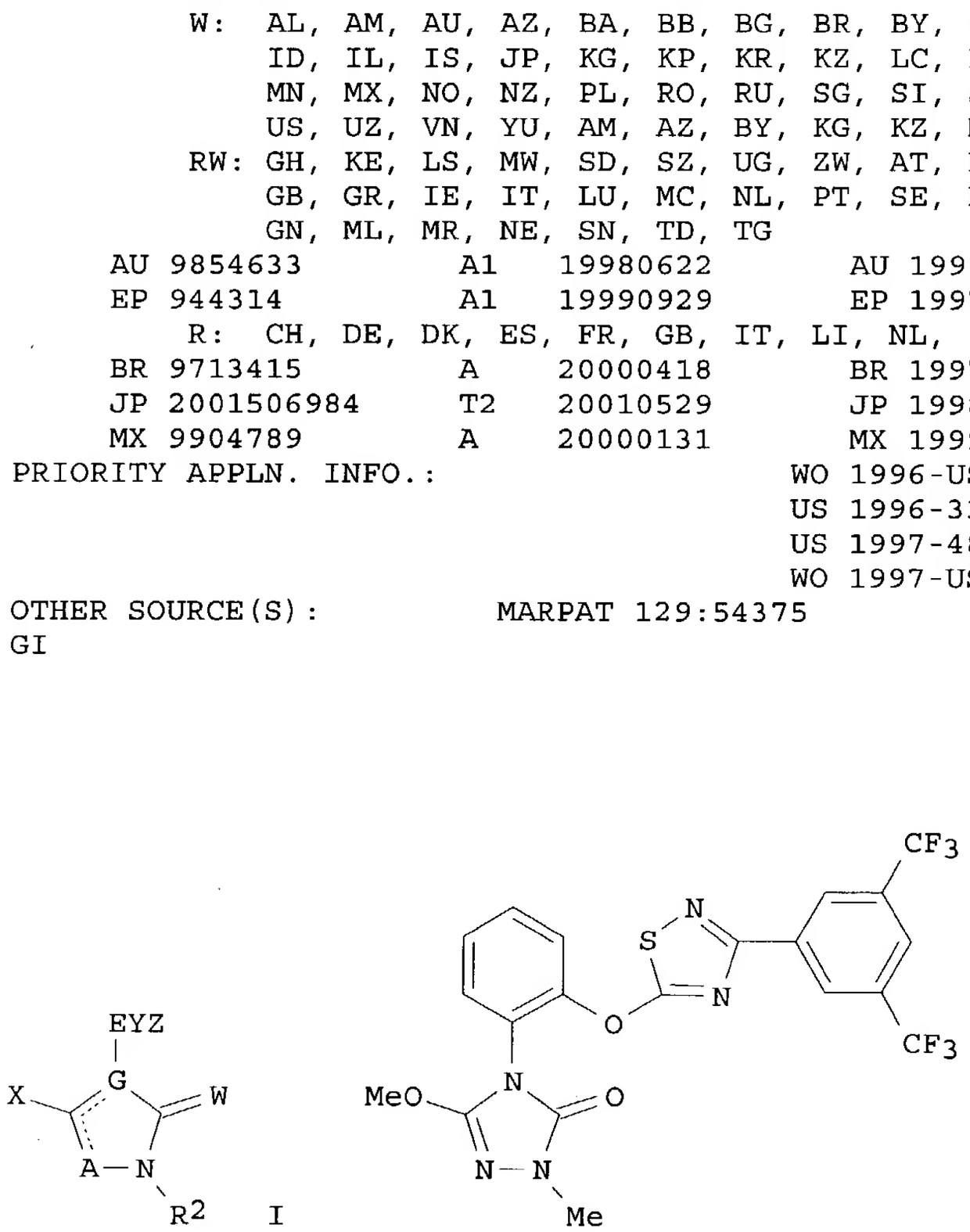
| | |
|---|---|
| | Alan; Selby, Thomas Paul |
| PATENT ASSIGNEE(S): | E. I. Du Pont de Nemours & Co., USA |
| SOURCE: | PCT Int. Appl., 232 pp. |
| | CODEN: PIXXD2 |
| DOCUMENT TYPE: | Patent |
| LANGUAGE: | English |
| FAMILY ACC. NUM. COUNT: | 2 |
| PATENT INFORMATION: | |

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9823155 | A1 | 19980604 | WO 1996-US18916 | 19961126 |
| W: JP, KR | | | | |
| RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| ZA 9709943 | A | 19990505 | ZA 1997-9943 | 19971105 |
| WO 9823156 | A1 | 19980604 | WO 1997-US21944 | 19971125 |
| W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, ID, IL, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| AU 9854633 | A1 | 19980622 | AU 1998-54633 | 19971125 |
| EP 944314 | A1 | 19990929 | EP 1997-948597 | 19971125 |
| R: CH, DE, DK, ES, FR, GB, IT, LI, NL, IE | | | | |
| BR 9713415 | A | 20000418 | BR 1997-13415 | 19971125 |
| JP 2001506984 | T2 | 20010529 | JP 1998-524889 | 19971125 |
| MX 9904789 | A | 20000131 | MX 1999-4789 | 19990524 |

| | | | |
|---|---|---|---|
| PRIORITY APPLN. INFO.: | WO 1996-US18916 | A | 19961126 |
| | US 1996-33614P | P | 19961219 |
| | US 1997-48844P | P | 19970606 |
| | WO 1997-US21944 | W | 19971125 |

OTHER SOURCE(S): MARPAT 129:54375

GI

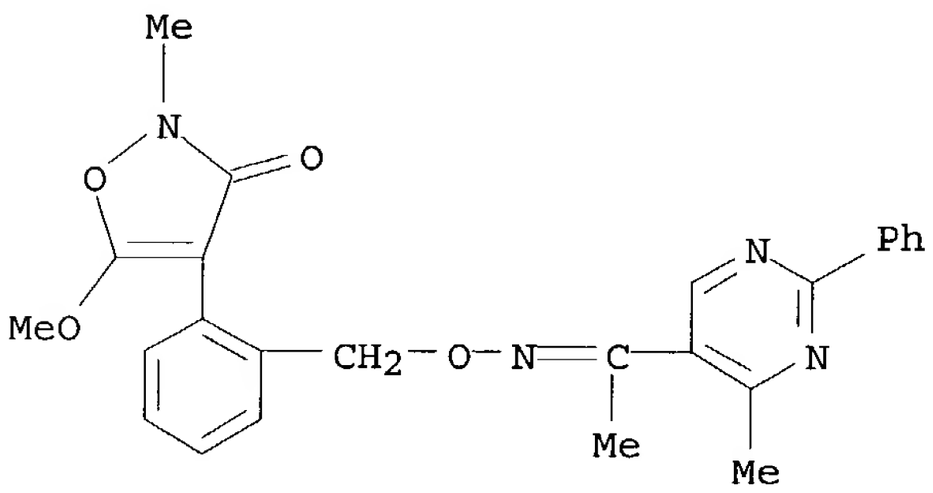



AB Title compds. I and their N-oxides and agriculturally suitable salts are disclosed [wherein E = (un)substituted 1,2-phenylene, naphthalene or heterocyclyl; A = O, S, N, NR3 or CR4; G = C or N; when G is C, then A is O, S or NR3 and the floating double bond is attached to G; and when G is N, than A is N or CR4 and the floating double bond is attached to A; W = O, S, NH, N(C1-C6 alkyl) or NO(C1-C6 alkyl); X = H, OR1, SOmR1, halo, C1-C6 alkyl, C1-C6 haloalkyl, C3-C6 cycloalkyl, cyano, NH2, NHR1, N(C1-C6 alkyl)R1, NH(C1-C6 alkoxy) or N(C1-C6 alkoxy)R1; R2 = H, C1-C6 alkyl, C1-C6 haloalkyl, C2-C6 haloalkyl, C2-C6 alkenyl, C2-C6 haloalkenyl, C2-C6

alkynyl, C2-C6 haloalkynyl, C3-C6 cycloalkyl, C2-C4 alkylcarbonyl, C2-C6 alkoxycarbonyl, hydroxy, C1-C2 alkoxy, or acetyloxy; R1= (halo)alkyl, (halo)alkenyl, etc.; R3= H, (halo)alkyl, etc.; Y = O, CO, SO, etc.; Z = (un)substituted alkyl, alkenyl or alkynyl, R4 = H, halo, alkyl, etc.; m = 0, 1 or 2]. Claims cover methods of arthropod and fungal control, novel compds., arthropodicidal and fungicidal compns., and novel intermediates. Approx. 1000 invention compds. were prepared For instance, 5-chloro-2,4-dihydro-4-(2-methoxyphenyl)-2-methyl-3H-1,2,4-triazol-3-one (preparation given) underwent a sequence of cleavage of the Me ether with BBr3, methoxylation of the chloride with NaOMe, and etherification of the phenolic hydroxy group with 5-chloro-3-[3,5-bis(trifluoromethyl) **phenyl**]-1,2,4-thiadiazole, to give title compound II. Selected I were active in screens against Erysiphe graminis, Pyricularia oryzae, Spodoptera frugiperda, Tetranychus urticae, and a variety of other standard pests.

IT **185336-64-5P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation as arthropodicide and fungicide)

RN 185336-64-5 CAPLUS
CN 3(2H)-Isoxazolone, 5-methoxy-2-methyl-4-[2-[[[[1-(4-methyl-2-phenyl-5-pyrimidinyl)ethylidene]amino]oxy]methyl]phenyl]- (9CI) (CA INDEX NAME)




REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 29 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:351919 CAPLUS
DOCUMENT NUMBER: 129:87956
TITLE: Color diffusion transfer image-forming system and color image formation
INVENTOR(S): Naruse, Hideaki; Nakamura, Takemare
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 82 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 10142764 | A2 | 19980529 | JP 1996-317058 | 19961113 |

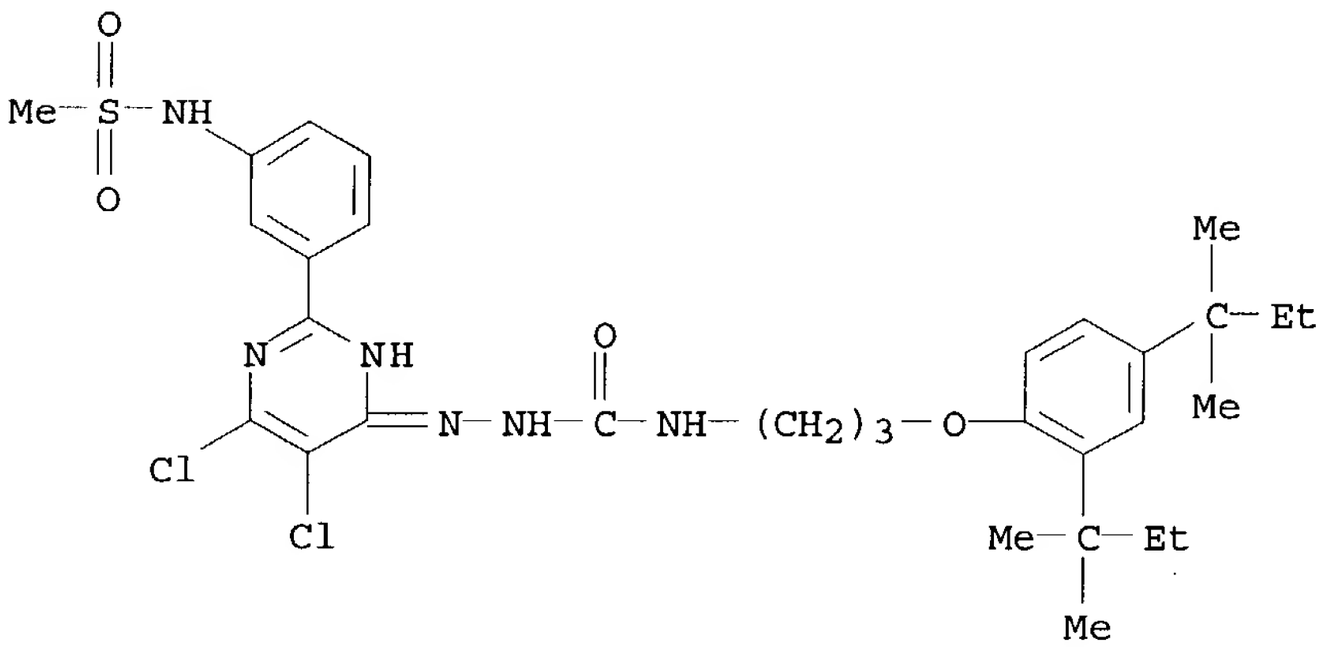
PRIORITY APPLN. INFO.: JP 1996-317058 19961113
OTHER SOURCE(S): MARPAT 129:87956
GI For diagram(s), see printed CA Issue.
AB In the title system using a photosensitive material containing a photosensitive Ag halide, a binder, a compound I (Z = carbamoyl, acyl,

alkoxycarbonyl, aryloxycarbonyl, sulfonyl, sulfamoyl; Q = atoms required to form an unsatd. ring along with the C atom), and a compound that reacts with an oxidized product of I to form or release a diffusive dye on a support and a dye-fixing material possessing ≥1 dye-fixing layer on which the dye formed by exposure and development of the photosensitive material is transferred, the dye-fixing layer and/or its adjacent layer contains ≥1 selected from phenol derivs., II and III [R10 = alkyl, alkenyl, aryl, aralkyl, heterocycle, R18CO, R19SO2, R20NHCO (R18-20 = substituent); R11, R12 = H, halo, alkyl, alkenyl, alkoxy, alkenoxy; R13-17 = H, alkyl, alkenyl, aryl; E = nonmetal atoms required to form a 5- to 7-membered ring along with the C and N atoms; R18 = H, alkyl, alkenyl, alkynyl, acyl, sulfonyl, sulfinyl, oxy radical, OH; R19-22 = H, alkyl]. The photosensitive material is imagewise exposed and laminated with the dye-fixing material followed by development to fix the diffusive dye from the photosensitive material on the dye-fixing material to form an image. Durable, high d. color images are obtained.

IT **209247-50-7**
RL: TEM (Technical or engineered material use); USES (Uses)
(diffusion-transfer photog. material containing hydrazine derivative color developer)

RN 209247-50-7 CAPLUS

CN Hydrazinecarboxamide, N-[3-[2,4-bis(1,1-dimethylpropyl)phenoxy]propyl]-2-[5,6-dichloro-2-[3-[(methylsulfonyl)amino]phenyl]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

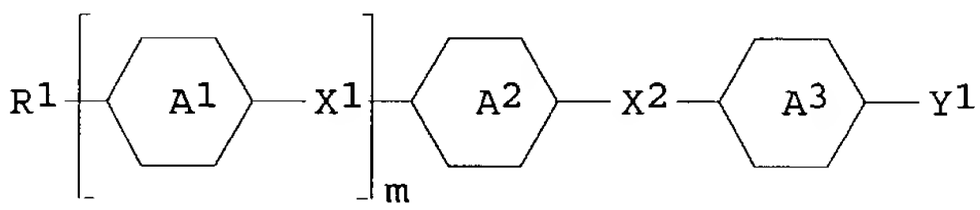


L11 ANSWER 30 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:341533 CAPLUS
DOCUMENT NUMBER: 129:21744
TITLE: **Phenyl** polyhaloalkyl ether derivatives, liquid-crystal composition containing the same, and liquid-crystal display element
INVENTOR(S): Shibata, Kouichi; Matsui, Shuichi; Miyazawa, Kazutoshi; Takeuchi, Hiroyuki; Hisatsune, Yasusuke; Takeshita, Fusayuki; Nakagawa, Etsuo
PATENT ASSIGNEE(S): Chisso Corp., Japan; Shibata, Kouichi; Matsui, Shuichi; Miyazawa, Kazutoshi; Takeuchi, Hiroyuki; Hisatsune, Yasusuke; Takeshita, Fusayuki; Nakagawa, Etsuo
SOURCE: PCT Int. Appl., 79 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

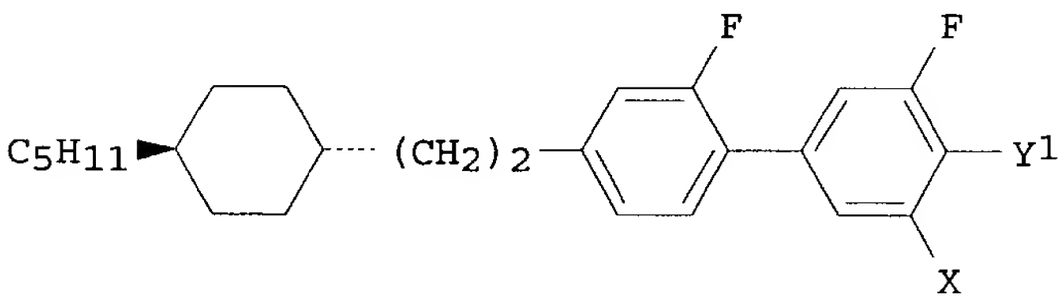
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9821172 | A1 | 19980522 | WO 1997-JP4114 | 19971112 |
| W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, ID, IL, IS, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| JP 10139709 | A2 | 19980526 | JP 1996-316958 | 19961113 |
| AU 9749642 | A1 | 19980603 | AU 1997-49642 | 19971112 |
| EP 945422 | A1 | 19990929 | EP 1997-912427 | 19971112 |
| R: DE, FR, GB | | | | |
| US 2001019121 | A1 | 20010906 | US 1999-308039 | 19990713 |

| PRIORITY APPLN. INFO.: | | | |
|---|---|---|---|
| | JP 1996-316958 | A | 19961113 |
| | WO 1997-JP4114 | W | 19971112 |

GI




I



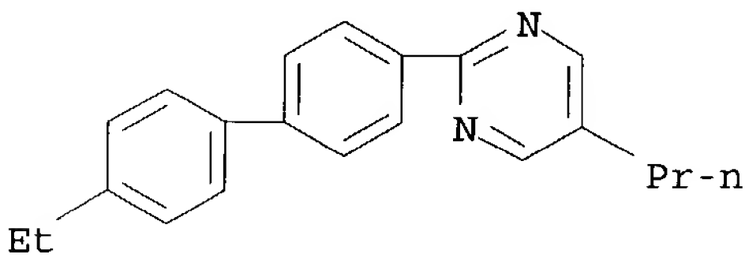

II

AB Claimed are novel liquid-crystal compds. which have an especially large value of dielec. anisotropy (Δε) and a satisfactory compatibility with other liquid-crystal compds. and show a nematic phase in a wide temperature range without detriment to the properties inherent in liquid-crystal fluorine compds.; a liquid-crystal composition containing the same; and a liquid-crystal display element prepared by using the composition The compds. include Ph polyhaloalkyl ether derivs. represented by general formula [I; wherein X1 and X2 each independently represents 1,2-ethylene, 1,4-butylene, or a covalent bond, provided that not both represent covalent bonds; R1 represents C1-20 alkyl in which at least one methylene group may have been replaced with oxygen, vinylene, or ethynylene; Y1 represents OCF2CFH(CF2)nF (wherein n is 0, 1, 2, or 3) or OCF2Cl; the rings A1 and A2 each independently represents 1,4-cyclohexylene, 1,4-cyclohexenylene, or 1,4-phenylene and A3 represents 1,4-phenylene, provided that at least one carbon atom in each ring may have been replaced with oxygen or nitrogen and at least one hydrogen atom present on each ring may have been replaced with fluorine or chlorine; m is 0 or 1; and each constituent element of the mol. may contain at least one of the isotopes thereof]. The liquid crystal display element is used for a watch, calculator, various instruments, automobile panel, word processor, electronic note, printer, computer, and TV. Thus, 2-fluoro-4-[2-(trans-4-pentylcyclohexyl)ethyl]boric acid (preparation given) was coupled with 3,5-difluoro-4-(1,1,2,3,3,3-hexafluoropropoxy)bromobenzene in the presence

of (Ph3P)4Pd and Na2CO3 in a mixture of toluene and water under reflux for 10 h to give the title compound (II; X = F, Y1 = OCF2CFHCF3), which showed phase transition temperature of C 41° N 99.5° I. A liquid crystal composition containing 85 weight% ZLI 1132 and 15 weight% II (X = H, Y1 = OCF2CF2H) showed TN1 at 73.5° and Δε of 10.6 vs. 83.7° and 8.3, resp., for II (X = H, Y1 = OCF2CF2H).

IT **175859-31-1**
RL: DEV (Device component use); PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
(liquid crystal composition containing; preparation of Ph polyhaloalkyl ether derivs., liquid-crystal composition containing them, and liquid-crystal display element)

RN 175859-31-1 CAPLUS
CN Pyrimidine, 2-(4'-ethyl[1,1'-biphenyl]-4-yl)-5-propyl- (9CI) (CA INDEX NAME)

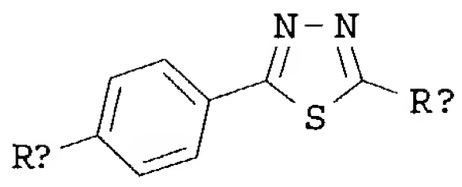



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

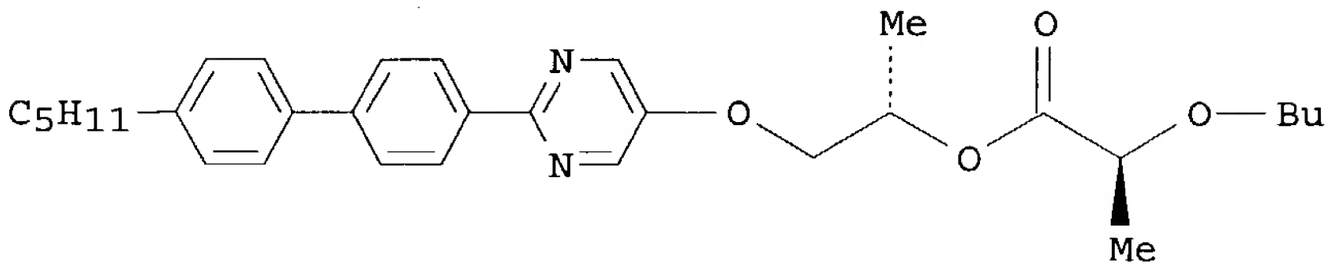
L11 ANSWER 31 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:323239 CAPLUS
DOCUMENT NUMBER: 128:315486
TITLE: Preparation of 2-(4-alkylphenyl)-5-alkylthiadiazoles as liquid crystals
INVENTOR(S): Saito, Shinichi; Shundo, Ryushi; Okabe, Eiji; Saito, Hideo
PATENT ASSIGNEE(S): Chisso Corp., Japan; Saito, Shinichi; Shundo, Ryushi; Okabe, Eiji; Saito, Hideo
SOURCE: PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9820004 | A1 | 19980514 | WO 1997-JP3896 | 19971027 |
| W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, ID, IL, IS, JP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| AU 9747245 | A1 | 19980529 | AU 1997-47245 | 19971027 |

PRIORITY APPLN. INFO.: JP 1996-307279 19961101
WO 1997-JP3896 19971027
OTHER SOURCE(S): MARPAT 128:315486
GI



I



II

AB The title 2-(4-alkylphenyl)-5-alkylthiadiazoles represented by general formula (I; Ra is C5-C15 alkyl; and Rb is C5-C15 alkyl) are prepared Claimed are ferroelec. liquid crystal compns. containing I. These compds. are liquid-crystal compds. which are usable as the basic substance of ferroelec. liquid crystal compns., have a low viscosity, and exhibit a liquid crystal phase in a low-temperature region. Thus, Et 4-octylbenzoate was sequentially condensed with hydrazine hydrate and octanoyl chloride to give N-(4-octylbenzoyl)-N'-octanoylhydrazine which was cyclocondensed with Lawesson's reagent to give I (Ra = octyl, Rb = heptyl) (II). II showed phase transition point (Cr 38° Sc 44.6° SA 51.3° Iso). A ferroelec. liquid crystal composition containing II (50 weight%) and a mixture of 6 phenylpyrimidine derivs. (45 weight%) and a chiral dopant (III) (5 weight%) showed phase transition point (room temperature-Sc* 54.4 SA 58.9 Iso) and response speed 30.0 μs at 44.4° in a liquid crystal cell (2 μm thickness).

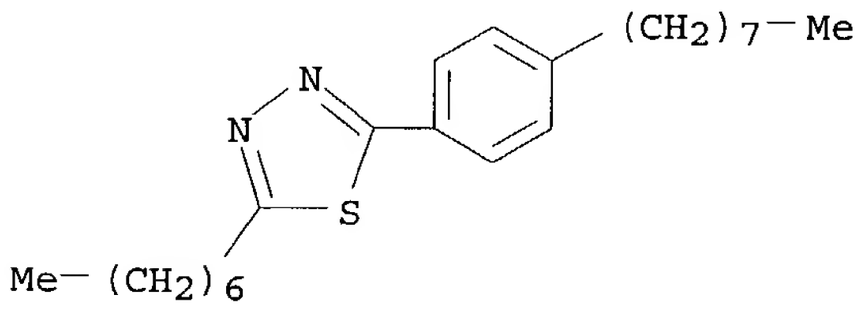
IT **206551-21-5**
RL: TEM (Technical or engineered material use); USES (Uses)
(preparation of (alkylphenyl)alkylthiadiazoles as liquid crystals for ferroelec. liquid crystal compns.)

RN 206551-21-5 CAPLUS

CN Propanoic acid, 2-butoxy-, (1S)-1-methyl-2-[[2-(4'-pentyl[1,1'-biphenyl]-4-yl)-5-pyrimidinyl]oxy]ethyl ester, (2S)-, mixt. with 2-[4-(decyloxy)phenyl]-5-octylpyrimidine, 2-(4'-heptyl[1,1'-biphenyl]-4-yl)-5-hexylpyrimidine, 5-heptyl-2-[4-(nonyloxy)phenyl]pyrimidine, 2-heptyl-5-(4-octylphenyl)-1,3,4-thiadiazole, 2-[4-(hexyloxy)phenyl]-5-octylpyrimidine, 5-hexyl-2-(4'-pentyl[1,1'-biphenyl]-4-yl)pyrimidine and 5-octyl-2-[4-(octyloxy)phenyl]pyrimidine (9CI) (CA INDEX NAME)

CM 1

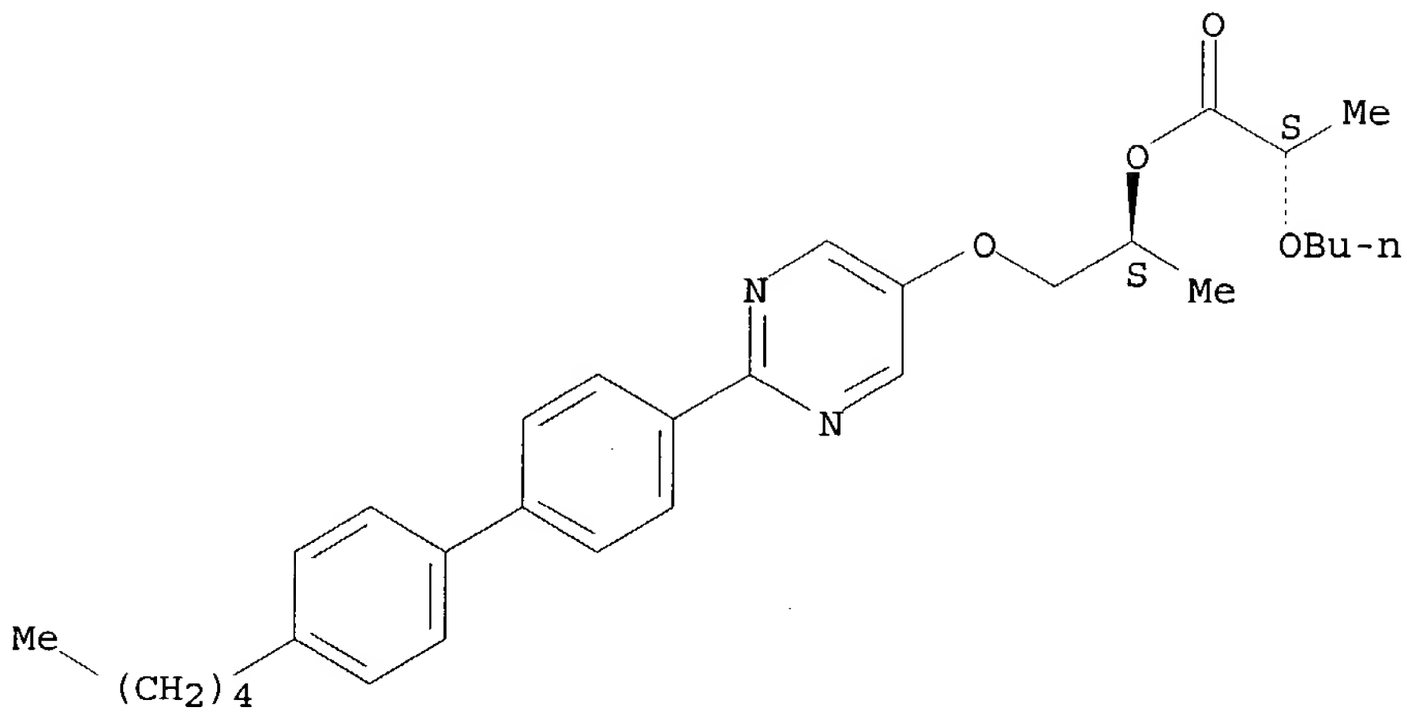
CRN 206550-94-9
CMF C23 H36 N2 S



CM 2

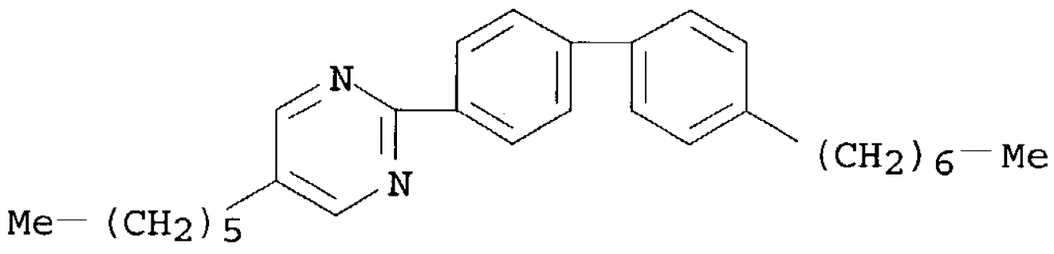
CRN 119218-09-6
CMF C31 H40 N2 O4

Absolute stereochemistry.



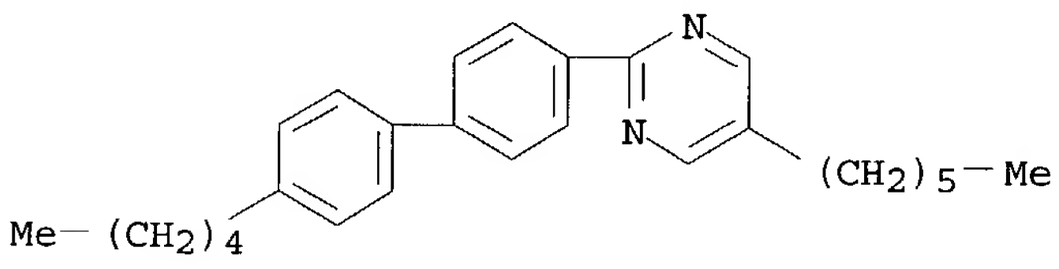

CM 3

CRN 92519-52-3
CMF C29 H38 N2



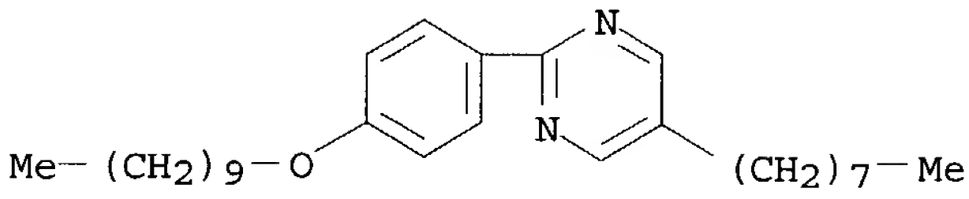

CM 4

CRN 92178-46-6
CMF C27 H34 N2



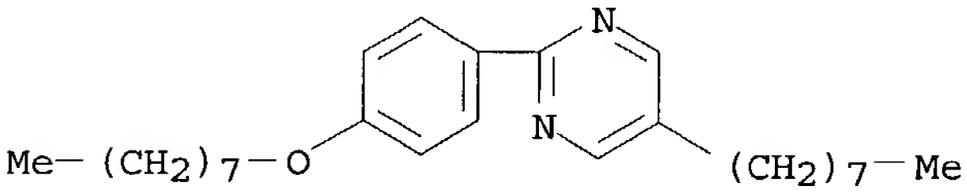

CM 5

CRN 57202-52-5
CMF C28 H44 N2 O



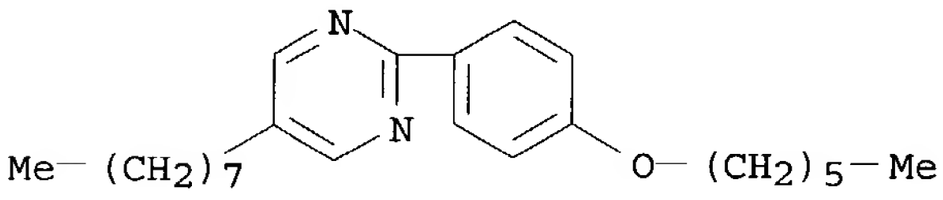
CM 6

CRN 57202-50-3
CMF C26 H40 N2 O



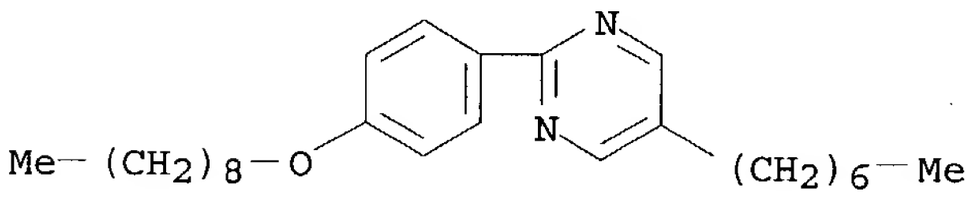
CM 7

CRN 57202-48-9
CMF C24 H36 N2 O



CM 8

CRN 57202-40-1
CMF C26 H40 N2 O



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 32 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:108200 CAPLUS
DOCUMENT NUMBER: 128:210966
TITLE: Manufacture of ferroelectric liquid-crystal composition for display
INVENTOR(S): Takiguchi, Takao; Nakamura, Shinichi; Utakawa, Masako
PATENT ASSIGNEE(S): Canon K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent

LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 10046149 | A2 | 19980217 | JP 1996-216983 | 19960731 |

PRIORITY APPLN. INFO.: JP 1996-216983 19960731

AB The manufacturing method involves the processes of (1) purifying ≥1 liquid-crystal compound by using 10-50 weight% (vs. the compound) active C and (2) mixing the purified compound with other components for the liquid-crystal composition The composition shows good switching property in a uniform state and gives high-contrast images.

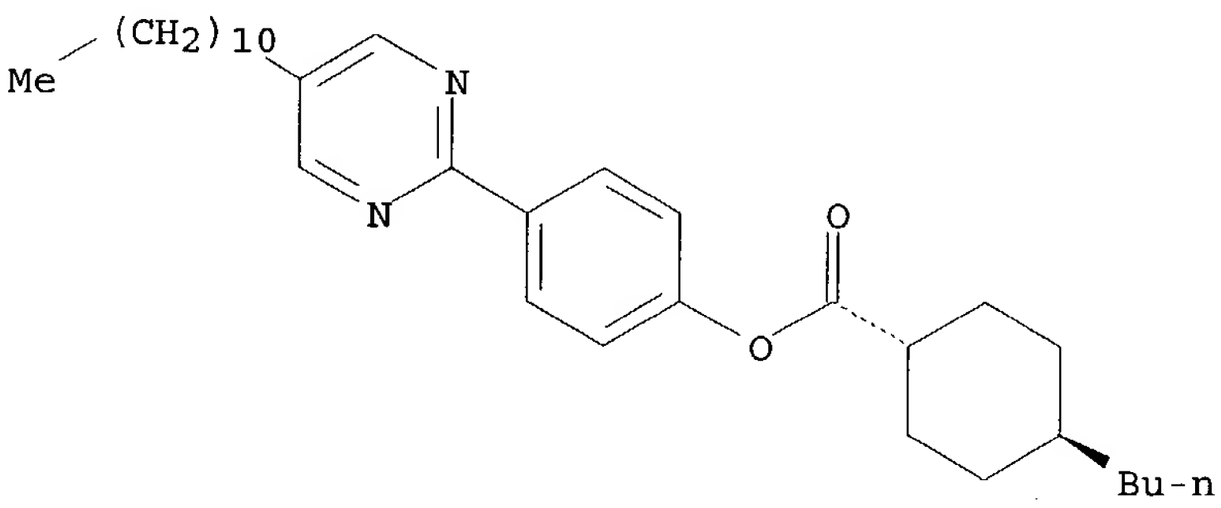
IT **204079-42-5**
RL: DEV (Device component use); USES (Uses)
(purification of liquid-crystal compound by active carbon in manufacture of ferroelec. liquid-crystal composition for display)

RN 204079-42-5 CAPLUS
CN Cyclohexanecarboxylic acid, 4-butyl-, 4-(5-undecyl-2-pyrimidinyl)phenyl ester, trans-, mixt. with 5-decyl-2-[4-[(2-fluorooctyl)oxy]phenyl]pyrimidine, 5-dodecyl-2-[4-[(2-fluorooctyl)oxy]phenyl]pyrimidine, 2-[4-(hexyloxy)phenyl]-5-nonylpyrimidine, 2-[4-(hexyloxy)phenyl]-5-octylpyrimidine, 2-[4-(nonyloxy)phenyl]-5-octylpyrimidine, trans-4-(5-undecyl-2-pyrimidinyl)phenyl 4-pentylcyclohexanecarboxylate and trans-4-(5-undecyl-2-pyrimidinyl)phenyl 4-propylcyclohexanecarboxylate (9CI) (CA INDEX NAME)

CM 1

CRN 121639-89-2
CMF C32 H48 N2 O2

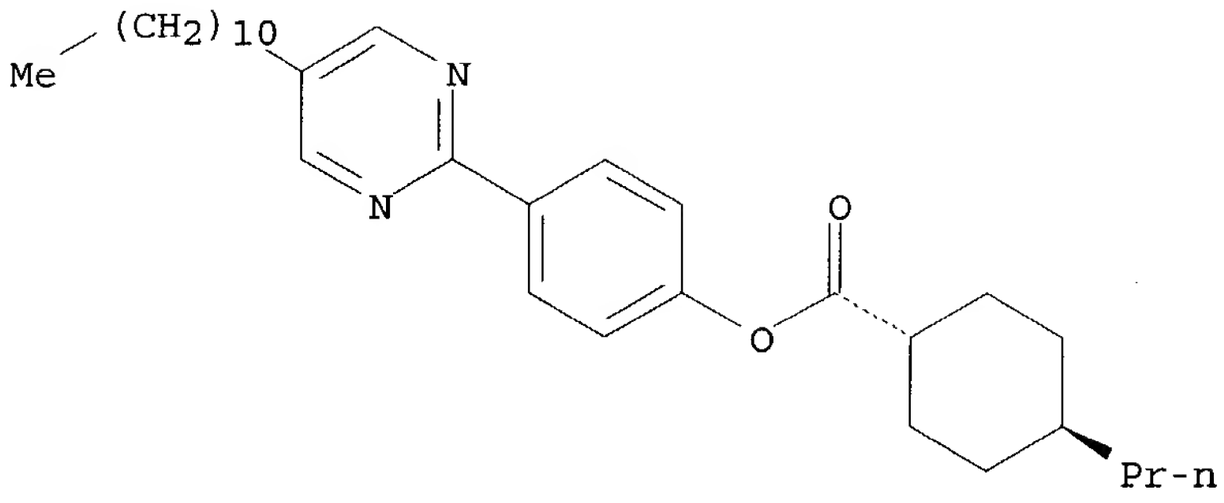
Relative stereochemistry.




CM 2

CRN 121639-88-1
CMF C31 H46 N2 O2

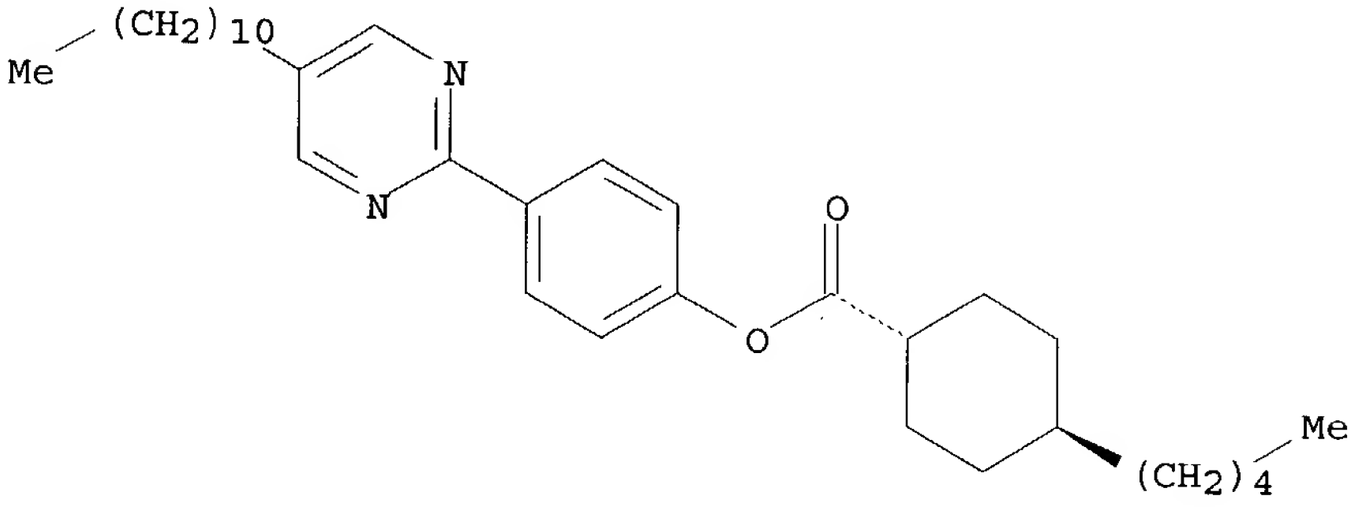
Relative stereochemistry.



CM 3

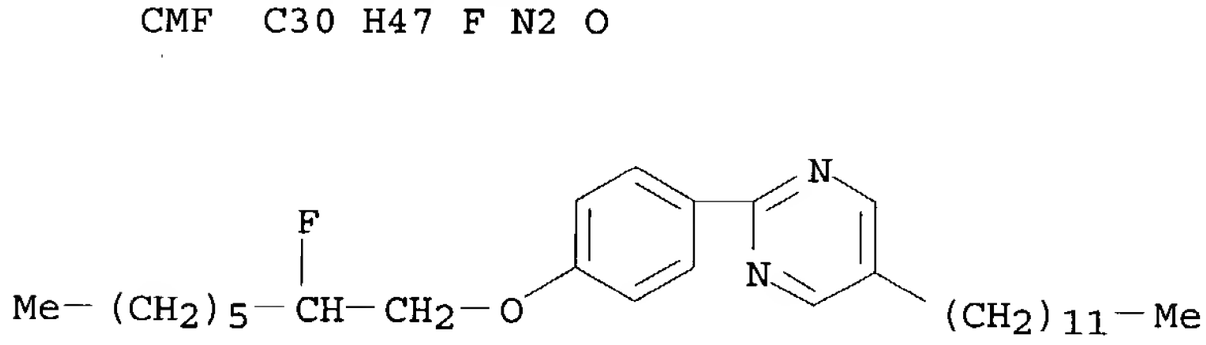
CRN 121083-94-1
CMF C33 H50 N2 O2

Relative stereochemistry.



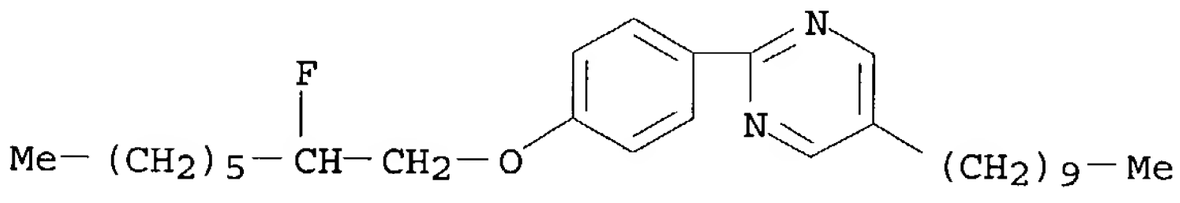
CM 4

CRN 116529-05-6
CMF C30 H47 F N2 O



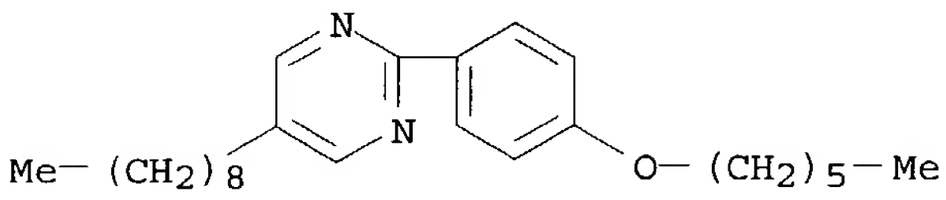
CM 5

CRN 113701-90-9
CMF C28 H43 F N2 O



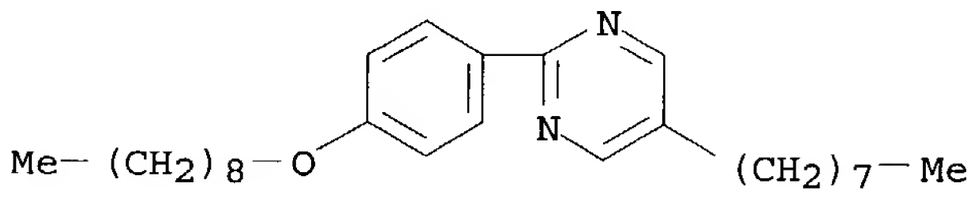
CM 6

CRN 57202-56-9
CMF C25 H38 N2 O



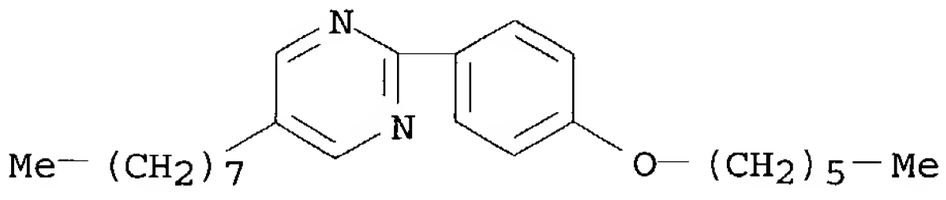
CM 7

CRN 57202-51-4
CMF C27 H42 N2 O



CM 8

CRN 57202-48-9
CMF C24 H36 N2 O

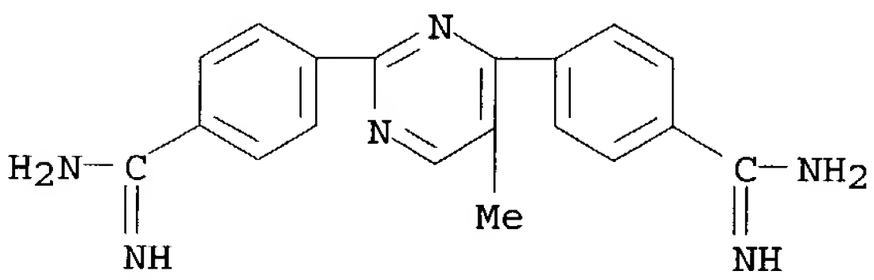


L11 ANSWER 33 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:90219 CAPLUS
DOCUMENT NUMBER: 128:225733
TITLE: Anti-Pneumocystis carinii pneumonia activity of dicationic diaryl methylpyrimidines
AUTHOR(S): Boykin, D. W.; Kumar, A.; Bajic, M.; Xiao, G.; Wilson, W. D.; Bender, B. C.; McCurdy, D. R.; Hall, J. E.; Tidwell, R. R.
CORPORATE SOURCE: Department of Chemistry and Center for Biotechnology and Drug Design, Georgia State University, Atlanta, GA, 30303-3083, USA
SOURCE: European Journal of Medicinal Chemistry (1997), 32(12), 965-972
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Editions Scientifiques et Medicales Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Synthesis of 2,4-bis(4-amidinophenyl)-5-methylpyrimidine 5, 2,4-bis[(4-imidazolin-2-yl)**phenyl**]-6-methylpyrimidine 5, 2,4-bis[(4-N-i-propylamidino)**phenyl**]-6-methylpyrimidine 7, and 2,4-bis[(4-N-isopentylamidino)**phenyl**]-6-methylpyrimidine 8 starting from 4-bromobenzamidien and 4'-bromoacetophenone is reported.

The synthesis of 2,4-bis-(4-amidinophenyl)-5-methylpyrimidine 12 and 2,4-bis-[(4-imidazolin-2-yl)**phenyl**]-5-methylpyrimidine 13, also beginning with 4-bromobenzamidine and 4'-bromo-propiophenone is described. A synthesis of 4,6-bis-(4-amidinophenyl)-2-methylpyrimidien 17, 4,6-bis-[(4-imidazolin-2-yl)**phenyl**]-2-methylpyrimidine 18, 4,6-bis[4-Ni-ipropylamidino)**phenyl**]-2-methylpyrimidine 19 and 4,6-bis[(4-N-n-propylamidino)**phenyl**]-2-methylpyrimidine 20 starting from acetamidine and 1,3-bis (4-bromophenyl)propenone is reported. Compds. 5-7 and 17-20 all bind strongly to the monor groove of poly-dA•dt whereas 8,12 and 13 bind less tightly as judged by their ΔTm values. A similar trend was noted for binding of these compds. to the 12-mer-d(CGCGAATTCGCG)2. Compds. 5,7 and 17 are more active and less toxic than pentamidine at its ED when evaluated against Pneumocystis carinii pneumonia (PCP) in the immunosuppressed rat model.

IT **160522-94-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(anti-pneumocystis carinii pneumonia activity of dicationic diaryl methylpyrimidines)

RN 160522-94-1 CAPLUS
CN Benzenecarboximidamide, 4,4'-(5-methyl-2,4-pyrimidinediyl)bis- (9CI) (CA INDEX NAME)




REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 34 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:21460 CAPLUS
DOCUMENT NUMBER: 128:121798
TITLE: Liquid crystal device and liquid crystal apparatus
INVENTOR(S): Tsuzuki, Hidetoshi; Kamio, Masaru; Okada, Shinjiro; Tsuboyama, Akira; Tokunaga, Hiroyuki; Tomono, Haruo; Sato, Koichi; Matsuo, Yuji; Katakura, Kazunori; Yokoyama, Yuko
PATENT ASSIGNEE(S): Canon Kabushiki Kaisha, Japan
SOURCE: Eur. Pat. Appl., 50 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 814142 | A2 | 19971229 | EP 1997-304210 | 19970616 |
| EP 814142 | A3 | 19981216 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| JP 10068923 | A2 | 19980310 | JP 1997-153664 | 19970611 |
| EP 1088877 | A2 | 20010404 | EP 2000-204626 | 19970616 |
| EP 1088877 | A3 | 20010411 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, | | | | |

IE, FI
US 6252641 B1 20010626 US 1997-874458 19970617
PRIORITY APPLN. INFO.: JP 1996-155503 A 19960617
JP 1997-153664 A 19970611
EP 1997-304210 A3 19970616
OTHER SOURCE(S): MARPAT 128:121798

AB A liquid crystal device is constituted by a pair of electrode plates and a liquid crystal composition disposed between the electrode plates. At least one of the electrode plates comprises a light-transmissive substrate, a plurality of electrodes including principal electrodes and auxiliary electrodes supported on the light-transmissive substrate, and an insulating layer. Each auxiliary electrode is disposed between an associated principal electrode and the light-transmissive substrate so as to be elec. connected with at least a part of the associated principal electrode, the auxiliary electrodes being disposed with spacings therebetween which are filled with the insulating layer. The liquid crystal composition comprises at least one species of a fluorine-containing mesomorphic compound comprising a fluorocarbon terminal portion and a hydrocarbon terminal portion, the terminal portions being connected with a central core and having smectic mesophase or latent smectic mesophase. The combination of the above specific cell structure and the specific liquid crystal composition is effective in improving display quality (e.g., contrast) while minimizing a voltage waveform deformation.

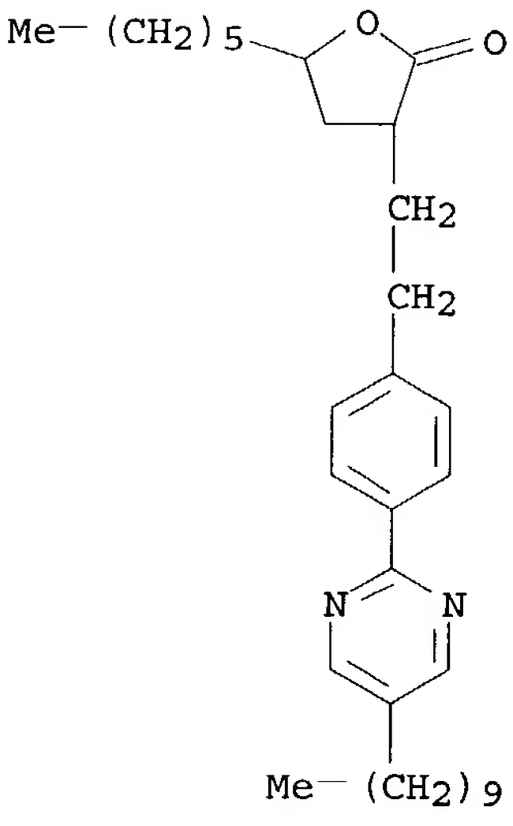
IT **173307-42-1**
RL: TEM (Technical or engineered material use); USES (Uses)
(liquid crystal composition for display devices)

RN 173307-42-1 CAPLUS

CN 2(3H)-Furanone, 3-[2-[4-(5-decyl-2-pyrimidinyl)phenyl]ethyl]-5-hexyldihydro-, mixt. with 5-decyl-2-[4-[(2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctyl)oxy]phenyl]pyrimidine, 2-[4-[2,2-difluoro-2-[1,1,2,2-tetrafluoro-2-(nonafluorobutoxy)ethoxy]ethoxy]phenyl]-5-octylpyrimidine, 5-nonyl-2-[4-[(2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctyl)oxy]phenyl]pyrimidine and 5-octyl-2-[4-[(2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctyl)oxy]phenyl]pyrimidine (9CI) (CA INDEX NAME)

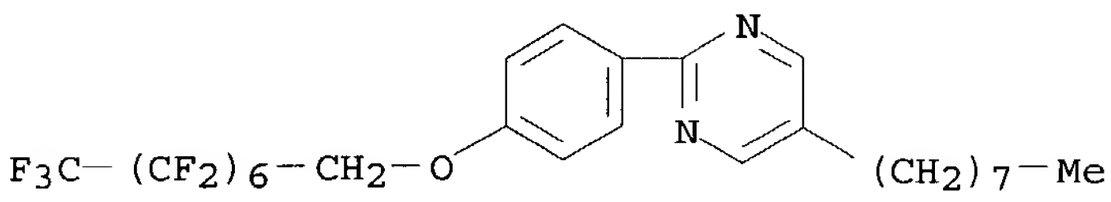
CM 1

CRN 170991-44-3
CMF C32 H48 N2 O2



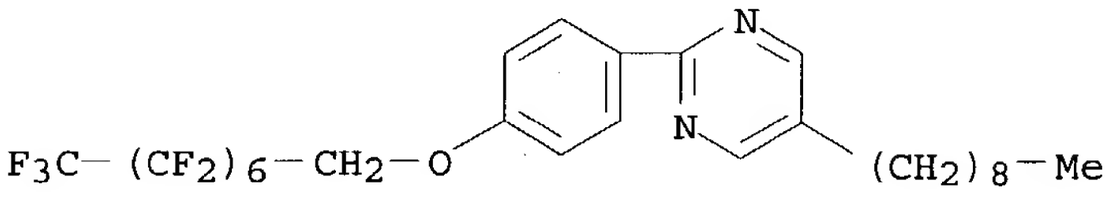
CM 2

CRN 152915-43-0
CMF C26 H25 F15 N2 O



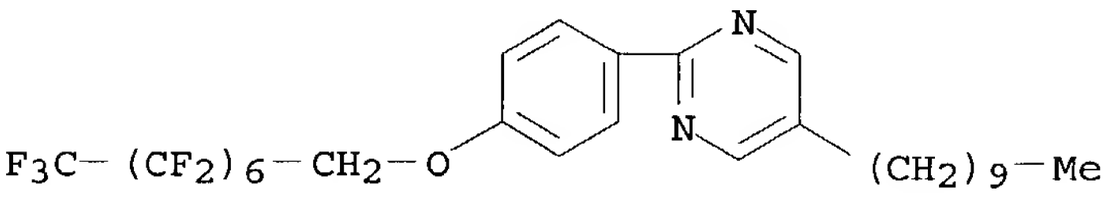
CM 3

CRN 152915-42-9
CMF C27 H27 F15 N2 O



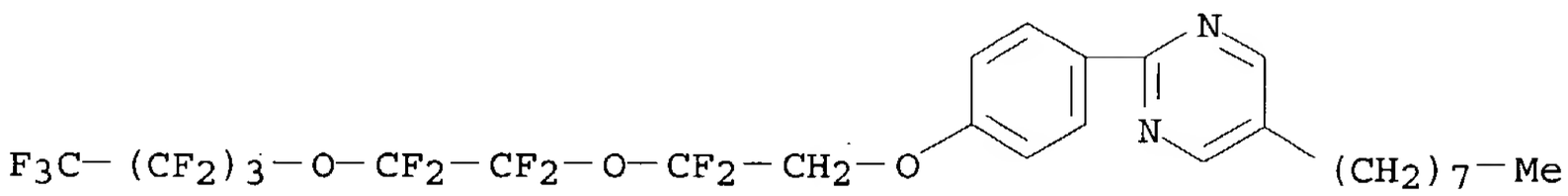
CM 4

CRN 152915-41-8
CMF C28 H29 F15 N2 O



CM 5

CRN 152914-98-2
CMF C26 H25 F15 N2 O3



L11 ANSWER 35 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:679042 CAPLUS
DOCUMENT NUMBER: 127:301549
TITLE: Preparation of liquid crystal compounds, liquid crystal compositions containing the compounds, and liquid crystal display devices made by using the compositions

09/ 811,359

INVENTOR(S): Ando, Tsugumichi; Matsui, Shuichi; Miyazawa, Kazutoshi; Takeuchi, Hiroyuki; Koizumi, Yasuyuki; Sekiguchi, Yasuko; Nakagawa, Etsuo; Takeshita, Fusayuki; et al.

PATENT ASSIGNEE(S): Chisso Corp., Japan; Ando, Tsugumichi; Matsui, Shuichi; Miyazawa, Kazutoshi; Takeuchi, Hiroyuki; Koizumi, Yasuyuki; Sekiguchi, Yasuko

SOURCE: PCT Int. Appl., 222 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

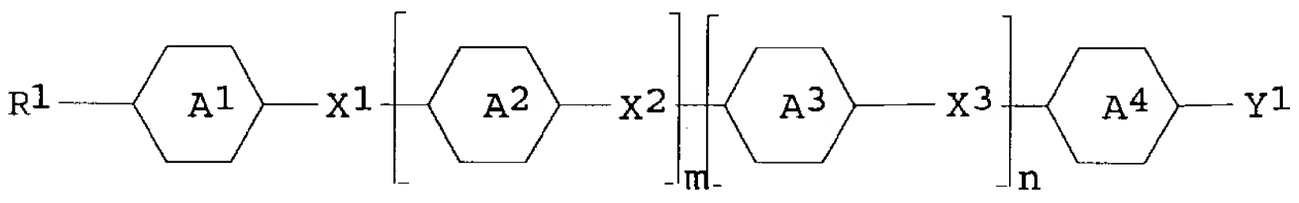
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9736847 | A1 | 19971009 | WO 1997-JP1048 | 19970327 |
| W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| AU 9720434 | A1 | 19971022 | AU 1997-20434 | 19970327 |
| EP 916639 | A1 | 19990519 | EP 1997-908523 | 19970327 |
| EP 916639 | B1 | 20020612 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE | | | | |
| CN 1218451 | A | 19990602 | CN 1997-194642 | 19970327 |
| CN 1118449 | B | 20030820 | | |
| EP 1043299 | A2 | 20001011 | EP 2000-113173 | 19970327 |
| EP 1043299 | A3 | 20040102 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE | | | | |
| JP 3231333 | B2 | 20011119 | JP 1997-535120 | 19970327 |
| JP 2002053529 | A2 | 20020219 | JP 2001-181798 | 19970327 |
| AT 219041 | E | 20020615 | AT 1997-908523 | 19970327 |
| TW 416979 | B | 20010101 | TW 1997-86104142 | 19970328 |
| US 6190576 | B1 | 20010220 | US 1998-155595 | 19980930 |
| US 6319570 | B1 | 20011120 | US 2000-597280 | 20000619 |

PRIORITY APPLN. INFO.:

| | | |
|---|---|---|
| JP 1996-79946 | A | 19960402 |
| JP 1996-239751 | A | 19960822 |
| EP 1997-908523 | A3 | 19970327 |
| JP 1997-535120 | A3 | 19970327 |
| WO 1997-JP1048 | W | 19970327 |
| US 1998-155595 | A1 | 19980930 |

OTHER SOURCE(S): MARPAT 127:301549

GI



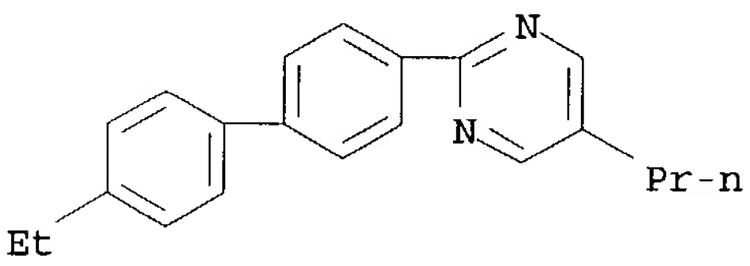

I

AB The above liquid crystal compds. represented by general formula (I; R1, Y1 = C1-20 alkyl; X1, X2, X3 = a single bond, 1,2-ethylene, vinylene, CO2, CF2O or OCF2; A1, A2, A3, A4 = trans-1,4-cyclohexylene or optionally fluorinated or chlorinated 1,4-phenylene, at least one of A2, A3 and A4 being 2,3-difluoro-1,4-phenylene; m, n = 0 or 1) with the proviso that the elements constituting the compds. may be each replaced by isotopes thereof are prepared Liquid crystal compns. containing the compds. I and liquid crystal

display devices made by using the compns. are claimed. These liquid crystal compds. are low in viscosity and high in dielec. anisotropy and have high specific resistance and high voltage retention, and are stable even when exposed to heat and UV rays. Thus, 2,3-difluoro-4-ethoxyphenol was condensed with 2-fluoro-4-[2-(trans-4-propylcyclohexyl)ethyl]benzoic acid using DCC in the presence of 4-dimethylaminopyridine at room temperature overnight to give 2,3-difluoro-4-ethoxyphenyl 2-fluoro-4-[2-(trans-4-propylcyclohexyl)ethyl]benzoate (II), which showed phase transition temperature 65.4° for C-N point and 141.3° for N-I point. A liquid crystal composition containing 15 weight% II and a mother liquid crystal composition (85 weight%) consisting of 4-butoxyphenyl 4-(trans-4-propylcyclohexyl)carboxybenzoate 27.6, 4-ethoxyphenyl 4-(trans-4-butylcyclohexyl)carboxybenzoate 20.7, 4-methoxyphenyl 4-(trans-4-pentylcyclohexyl)carboxybenzoate 20.7, 4-ethoxyphenyl 4-(trans-4-propylcyclohexyl)carboxybenzoate 17.2, and 4-ethoxyphenyl 4-(trans-4-pentylcyclohexyl)carboxybenzoate 13.8 weight% showed clearing point 129.4° and dielec. anisotropy (Δε) -4.17 as compared to 74.6° and 0.0, resp., for the mother liquid crystal composition

IT **175859-31-1**
RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)
(liquid crystal composition containing; preparation of liquid crystal compds., liquid crystal compns. containing the compds., and liquid crystal display devices made by using them)

RN 175859-31-1 CAPLUS
CN Pyrimidine, 2-(4'-ethyl[1,1'-biphenyl]-4-yl)-5-propyl- (9CI) (CA INDEX NAME)



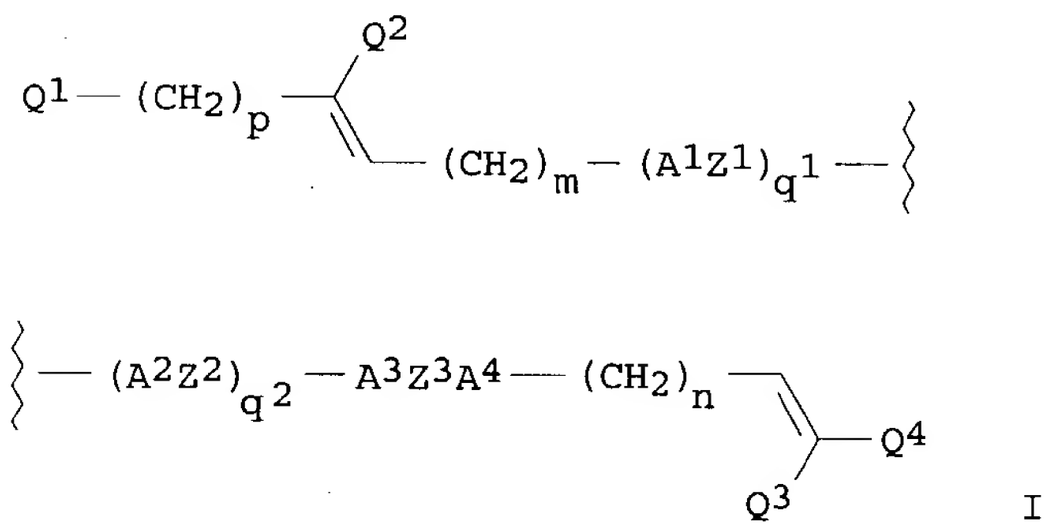

L11 ANSWER 36 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:640630 CAPLUS
DOCUMENT NUMBER: 127:339303
TITLE: Bialkenyl derivatives, liquid crystalline compounds and liquid crystal compositions
INVENTOR(S): Kato, Takashi; Matsui, Shuichi; Miyazawa, Kazutoshi; Sekiguchi, Yasuko; Nakagawa, Etsuo
PATENT ASSIGNEE(S): Chisso Corp., Japan; Kato, Takashi; Matsui, Shuichi; Miyazawa, Kazutoshi; Sekiguchi, Yasuko; Nakagawa, Etsuo
SOURCE: PCT Int. Appl., 116 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9734855 | A1 | 19970925 | WO 1997-JP700 | 19970306 |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, KE, KG, KR, KZ, LC, LK, LR, | | | | |

LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

| | | | | | |
|---|---|---|---|---|---|
| JP 10045639 | A2 | 19980217 | JP 1997-24331 | 19970123 | |
| AU 9722324 | A1 | 19971010 | AU 1997-22324 | 19970306 | |
| EP 891314 | A1 | 19990120 | EP 1997-905457 | 19970306 | |
| EP 891314 | B1 | 20010905 | | | |
| R: DE, FR, GB | | | | | |
| CN 1214036 | A | 19990414 | CN 1997-193138 | 19970306 | |
| CN 1110470 | B | 20030604 | | | |
| US 6180027 | B1 | 20010130 | US 1998-101990 | 19980722 | |

PRIORITY APPLN. INFO.: JP 1996-90585 A 19960318
WO 1997-JP700 W 19970306
OTHER SOURCE(S): MARPAT 127:339303
GI

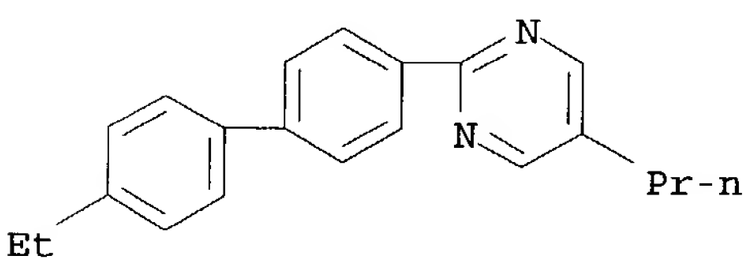


I

AB Liquid crystalline compds. expressed by formula I (A1-4 = trans-1,4-cyclohexylene, etc.; Z1-3 = (CH2)2, etc.; Q1-2 = H, F, Cl, Br; Q3-4 = F, Cl, Br; m,n,p = integer 0-5; q1-q2 = integer 0-1), liquid crystal compns. thereof obtained by combination with specified liquid crystal compds., and liquid crystal display devices using them are disclosed. The compns. provide a wide liquid crystal phase temperature range.

IT **175859-31-1**
RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)
(electrooptical display devices using liquid crystal compns. containing)

RN 175859-31-1 CAPLUS
CN Pyrimidine, 2-(4'-ethyl[1,1'-biphenyl]-4-yl)-5-propyl- (9CI) (CA INDEX NAME)



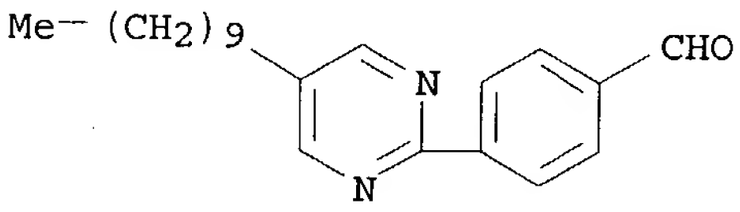
L11 ANSWER 37 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:590496 CAPLUS

09/ 811,359

DOCUMENT NUMBER: 127:247916
TITLE: Formylation of triflates by carbon monoxide and hydrosilanes
INVENTOR(S): Kotsuki, Hikizo; Suenaga, Hitoshi; Datta, Peobal kanti
PATENT ASSIGNEE(S): Teikoku Hormone Mfg. Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 09227439 | A2 | 19970902 | JP 1996-75107 | 19960222 |

PRIORITY APPLN. INFO.: JP 1996-75107 19960222
OTHER SOURCE(S): CASREACT 127:247916
AB Triflates are formylated using CO as a C source and hydrosilanes as proton sources in the presence of catalysts. 4-Me3CC6H4O3SCF3 was treated with CO in DMF in the presence of Pd(OAc)2 and 1,3-bis(diphenylphosphino)propane at 70° for 20 min and treated with trioctylsilane and NEt3 at 70° to give 89% 4-Me3CC6H4CHO.
IT **177581-96-3P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(formylation of triflates by CO and hydrosilanes)
RN 177581-96-3 CAPLUS
CN Benzaldehyde, 4-(5-decyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)




L11 ANSWER 38 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:299249 CAPLUS
DOCUMENT NUMBER: 126:285791
TITLE: Liquid crystalline compound substituted with fluorine containing group, liquid crystal composition, and liquid crystal display device
INVENTOR(S): Miyazawa, Kazutoshi; Matsui, Shuichi; Kondo, Tomoyuki; Kato, Takashi; Sekiguchi, Yasuko; Nakagawa, Etsuo
PATENT ASSIGNEE(S): Chisso Corp., Japan
SOURCE: Eur. Pat. Appl., 58 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

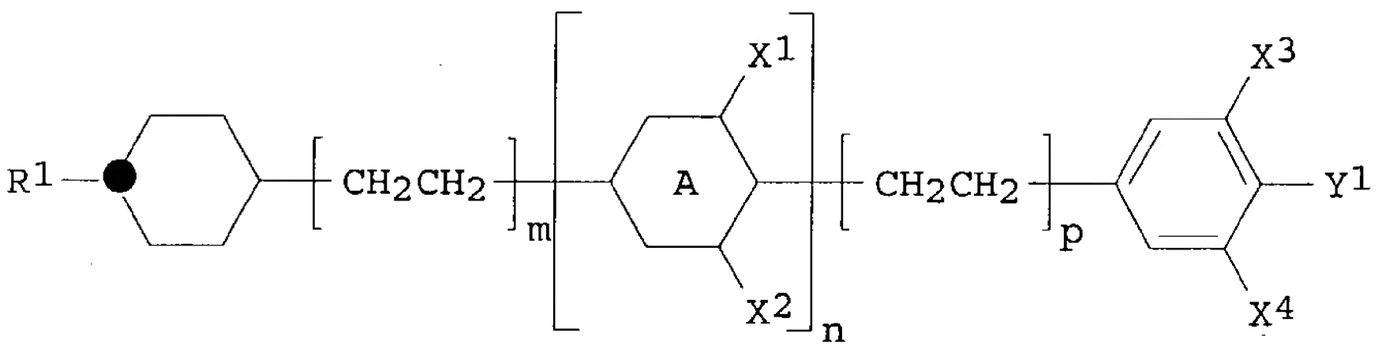
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 761799 | A1 | 19970312 | EP 1996-113195 | 19960816 |
| R: CH, DE, FR, GB, LI | | | | |
| JP 09137162 | A2 | 19970527 | JP 1995-319515 | 19951114 |
| JP 09137163 | A2 | 19970527 | JP 1995-319516 | 19951114 |
| JP 09137164 | A2 | 19970527 | JP 1995-319517 | 19951114 |
| JP 2896648 | B2 | 19990531 | | |
| TW 426723 | B | 20010321 | TW 1996-85107358 | 19960618 |

| | | | | |
|---|---|---|---|---|
| US 5948318 | A | 19990907 | US 1996-698456 | 19960815 |
| US 6117360 | A | 20000912 | US 1996-698451 | 19960815 |
| CN 1153807 | A | 19970709 | CN 1996-111984 | 19960910 |

PRIORITY APPLN. INFO.: JP 1995-258185 A 19950911
JP 1995-319517 A 19951114

OTHER SOURCE(S): MARPAT 126:285791

GI



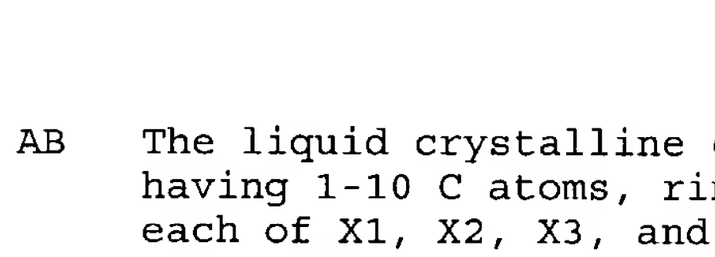
I

AB The liquid crystalline compds. I are given wherein R1 represents an alkyl group having 1-10 C atoms, ring A represents 1,4-phenylene or 1,4-cyclohexylene, each of X1, X2, X3, and X4 independently represents H atom or F atom, Y1 represents CF3 or OCF3, and each of m, n, and p is independently an integer of 1 or 0. The liquid crystalline compds. have a wide temperature range of nematic phase, low viscosity, large pos. Δε, high chemical stability, high miscibility with other liquid crystalline compds. at low temps., small temperature dependency of viscosity and Δε, extremely high specific resistance (high voltage holding ratio), and good UV stability, and are preferably used for TFT. Also, disclosed are liquid crystal compns. containing the liquid crystalline compds. mentioned above, and liquid crystal display devices using the liquid crystal composition

IT **148832-61-5D**, mixture containing
RL: TEM (Technical or engineered material use); USES (Uses)
(liquid crystal)

RN 148832-61-5 CAPLUS

CN Pyrimidine, 5-ethyl-2-(4'-ethyl[1,1'-biphenyl]-4-yl)- (9CI) (CA INDEX NAME)



L11 ANSWER 39 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

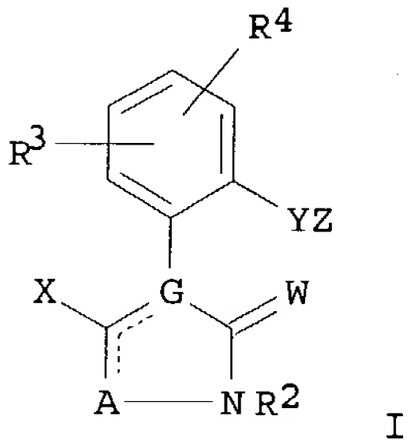
| | |
|---|---|
| ACCESSION NUMBER: | 1997:51535 CAPLUS |
| DOCUMENT NUMBER: | 126:74854 |
| TITLE: | Preparation of arylazolones as agrochemical fungicides. |
| INVENTOR(S): | Brown, Richard James; Sun, King-Mo; Frasier, Deborah Ann |
| PATENT ASSIGNEE(S): | E. I. Du Pont de Nemours & Co., USA; Brown, Richard James; Sun, King-Mo; Frasier, Deborah Ann |
| SOURCE: | PCT Int. Appl., 95 pp.<br>CODEN: PIXXD2 |
| DOCUMENT TYPE: | Patent |
| LANGUAGE: | English |
| FAMILY ACC. NUM. COUNT: | 1 |

09/ 811,359

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9636615 | A1 | 19961121 | WO 1995-US5847 | 19950516 |
| W: JP, KR, US | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| JP 10504042 | T2 | 19980414 | JP 1995-534772 | 19950516 |

PRIORITY APPLN. INFO.: WO 1995-US5847 19950516
OTHER SOURCE(S): MARPAT 126:74854
GI



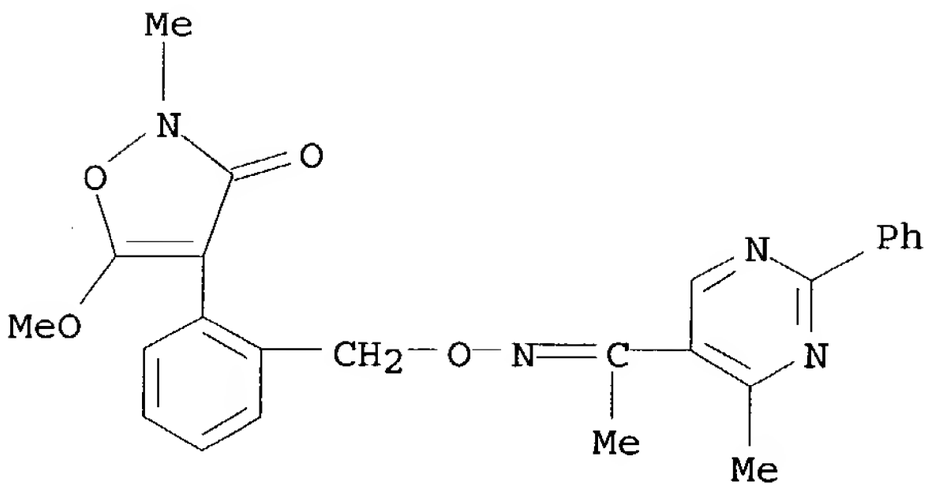

I

AB Title compds. [I; A = O, S, N, NR5, CR14; G = C, N; W = O, S; X = OR1, SR1, SOR1, SO2R1, halo; R1 = alkyl, haloalkyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl, cycloalkyl, alkylcarbonyl, alkoxycarbonyl, (substituted) PhCO; R2, R5 = H, R1; R3, R4 = H, halo, cyano, NO2, alkyl, haloalkyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl, alkoxy, haloalkoxy, alkenyloxy, alkynyloxy; Y O, S, SO, SO2, CHR6O, CHR6ON:CR7, C.tplbond.C, bond, etc.; R6 = H, alkyl; R7 = H, alkyl, haloalkyl, alkoxy, haloalkoxy, alkenyl, haloalkenyl, alkynyl, haloalkynyl, cycloalkyl, alkylcarbonyl, alkoxycarbonyl, cyano, morpholino; R14 = H, halo, alkyl, haloalkyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl, cycloalkyl; Z = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, Ph, (aromatic) heterocyclyl, etc.; with provisos], were prepared Thus, o-tolyl isocyanate reacted with Me2NNH2 in PhMe to give 2,2-dimethyl-N-(2-methylphenyl)hydrazinecarboxamide. This was refluxed with triphosgene in CH2Cl2 to give 5-chloro-2,4-dihydro-2-methyl-4-(2-methylphenyl)-3H-1,2,4-triazol-3-one, which was converted to 2,4-dihydro-5-methoxy-2-methyl-4-[2-[[(phenylmethylene)amine]oxy]methyl] **phenyl**-3H-1,2,4-triazol-3-one. Several title compds. gave complete control of Erysiphe graminis, Puccinia recondita, and Plasmopara viticola.

IT **185336-64-5P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of arylazolones as agrochem. fungicides)

RN 185336-64-5 CAPLUS

CN 3(2H)-Isoxazolone, 5-methoxy-2-methyl-4-[2-[[[[1-(4-methyl-2-phenyl-5-pyrimidinyl)ethylidene]amino]oxy]methyl]phenyl]- (9CI) (CA INDEX NAME)

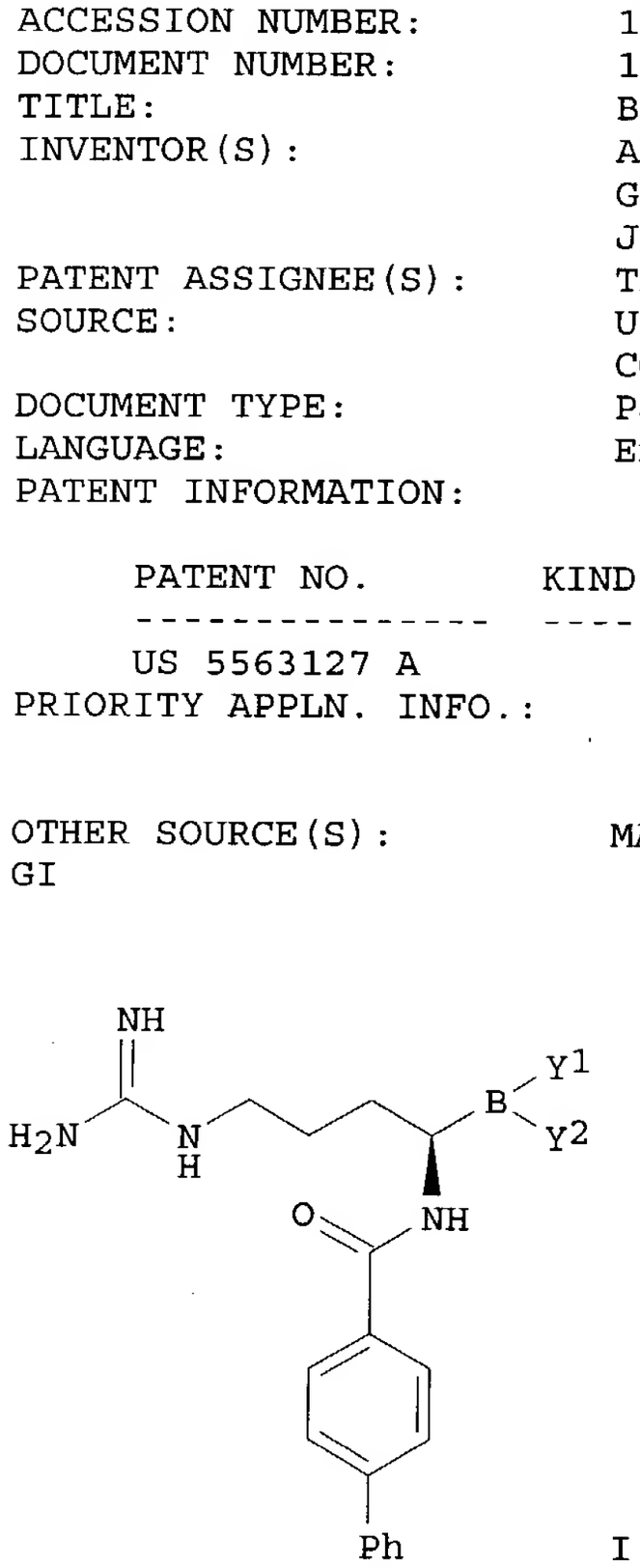


L11 ANSWER 40 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:672852 CAPLUS
DOCUMENT NUMBER: 126:31466
TITLE: Boronic acid and ester inhibitors of thrombin
INVENTOR(S): Amparo, Eugene C.; Miller, William H.; Pacofsky, Gregory J.; Wityak, John; Weber, Patricia C.; Duncia, John J. V.; Santella, Joseph B., III
PATENT ASSIGNEE(S): The Dupont Merck Pharmaceutical Company, USA
SOURCE: U.S., 170 pp., Cont.-in-part of U.S. Ser. No. 348,029.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 5563127 A | | 19961008 | US 1994-364338 | 19941227 |
| PRIORITY APPLN. INFO.: | | | US 1993-36377 | 19930324 |
| | | | US 1994-318029 | 19941004 |
| | | | US 1994-348029 | 19941201 |

OTHER SOURCE(S): MARPAT 126:31466
GI



I

AB Novel boronic acid and ester and carboxyl-modified amino acid compds. R1-Z-CHR2-A (A = organoboryl, BY1Y2; Y1, Y2 = independently OH, F, organoamino, C1-8 alkoxy, Y1Y2 = cyclic boron ester, amide containing N, S, O; etc.; Z = (CH2)mCX, X = amido, thioamido, etc., substituted C1-12 alkyl, alkenyl, etc.; R1 = arylalkenyl, aryl = substituted Ph, **naphthyl**, biphenyl, etc.; R2 = substituted C1-12 alkyl, alkenyl, etc.), which are inhibitors of trypsin-like enzymes, are disclosed. Thus, amino acid modified boronic ester I (Y1Y2 = (+)-pinanediol) was prepared in multiple

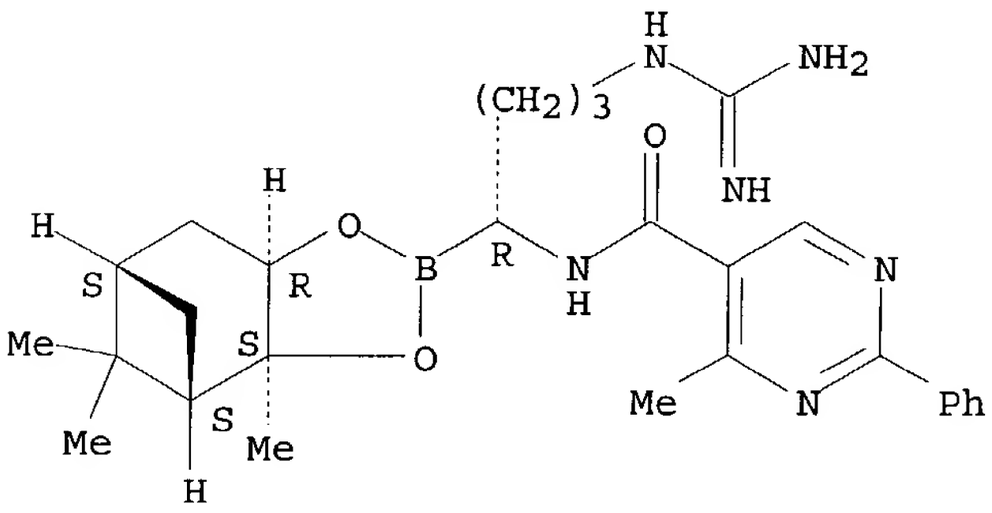
steps starting from (+)-pinanediol 4-bromo-1(R)-(4-phenylbenzoyl)aminobutane-1-boronate. Thrombin inhibition activity of some of the compds. prepared is described.

IT **180896-93-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amino acid-modified boronic acids and esters as inhibitors of thrombin)

RN 180896-93-9 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[(1R)-4-[(aminoiminomethyl)amino]-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]butyl]-4-methyl-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




L11 ANSWER 41 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:466907 CAPLUS

DOCUMENT NUMBER: 125:127905

TITLE: Ethynylene compound for liquid-crystal composition and liquid-crystal display element using same

INVENTOR(S): Takiguchi, Takao; Iwaki, Takashi; Tokano, Goji; Yamada, Yoko; Nakamura, Shinichi

PATENT ASSIGNEE(S): Canon Kk, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 35 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 08109145 | A2 | 19960430 | JP 1994-271847 | 19941012 |

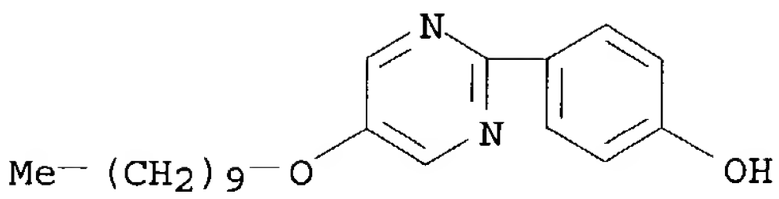
PRIORITY APPLN. INFO.: JP 1994-271847 19941012

AB Claimed is an ethynylene compound such as 1-(5-decyloxypyrimidine-2-yl)-4-(4-**phenyl**-1-butynyl)benzene. A liquid-crystal composition contains an ethynylene compound, and a liquid-crystal display element comprises the above liquid-crystal composition layer enclosed between a pair of electrode substrates.

IT **110203-06-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ethynylene compound for liquid-crystal composition from)

RN 110203-06-0 CAPLUS

CN Phenol, 4-[5-(decyloxy)-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



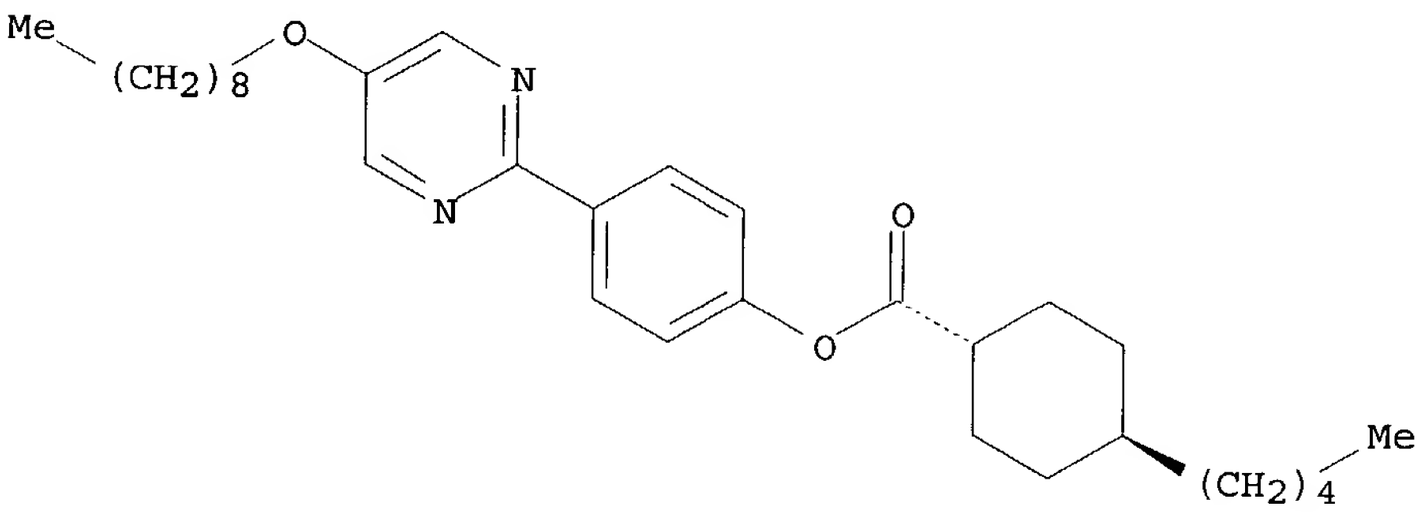
L11 ANSWER 42 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:353352 CAPLUS
DOCUMENT NUMBER: 124:356726
TITLE: Synthesis and mesomorphic properties of fluorinated liquid crystals obtained from optically active 2-fluoro-octanol
AUTHOR(S): Liu, Hong; Nohira, Hiroyuki
CORPORATE SOURCE: Dep. Applied Chem., Saitama Univ., Urawa, 338, Japan
SOURCE: Liquid Crystals (1996), 20(5), 581-586
CODEN: LICRE6; ISSN: 0267-8292
PUBLISHER: Taylor & Francis
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Several homologs of semi-fluorinated liquid crystals, 4'-[(n-perfluoroalkyl)alkyloxy]**phenyl** 4-(2-fluorooctyloxy)benzoates and 4'-(2-fluorooctyloxy)**phenyl** 4-[(n-perfluoroalkyl)alkyloxy]benzoates were synthesized. One set of the compds., with the central carbonyl group conjugated to the terminal position carrying the nonchiral perfluoroalkyloxy tail, showed enhanced chiral smectic C behavior, while the other set, with the central carbonyl group conjugated to the terminal position carrying the chiral 2-fluoro-octyloxy tail, exhibited enhanced smectic A behavior. The mesomorphic properties of these novel fluorinated materials are reported and the effects of extent of fluorination are discussed.

IT **122893-54-3**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(liquid crystal properties of phenylpyrimidine mixture doped with (fluorooctyl)(perfluoroalkylalkoxy)benzenes)

RN 122893-54-3 CAPLUS
CN Cyclohexanecarboxylic acid, 4-pentyl-, 4-[5-(nonyloxy)-2-pyrimidinyl]phenyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L11 ANSWER 43 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:253101 CAPLUS
DOCUMENT NUMBER: 125:32885
TITLE: An efficient procedure for palladium-catalyzed hydroformylation of aryl/enol triflates

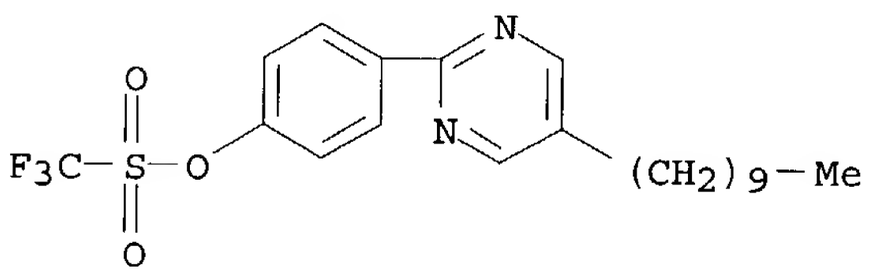
09/ 811,359

AUTHOR(S): Kotsuki, Hiyoshizo; Datta, Probal Kanti; Suenaga, Hitoshi
CORPORATE SOURCE: Faculty Science, Kochi Univ., Kochi, 780, Japan
SOURCE: Synthesis (1996), (4), 470-2
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:32885

AB An efficient method for hydroformylation of aryl and enol trifluoromethanesulfonates is presented. Their reaction with CO, trioctylsilane, and Et3N in the presence of a catalytic amount of Pd(OAc)2 and 1,3-bis(diphenylphosphanyl)propane proceeds efficiently to provide a variety of aromatic and α,β-unsatd. aldehydes.

IT **173346-92-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aromatic and α,β-unsatd. aldehydes by palladium-catalyzed hydroformylation of aryl/enol triflates)

RN 173346-92-4 CAPLUS
CN Methanesulfonic acid, trifluoro-, 4-(5-decyl-2-pyrimidinyl)phenyl ester (9CI) (CA INDEX NAME)



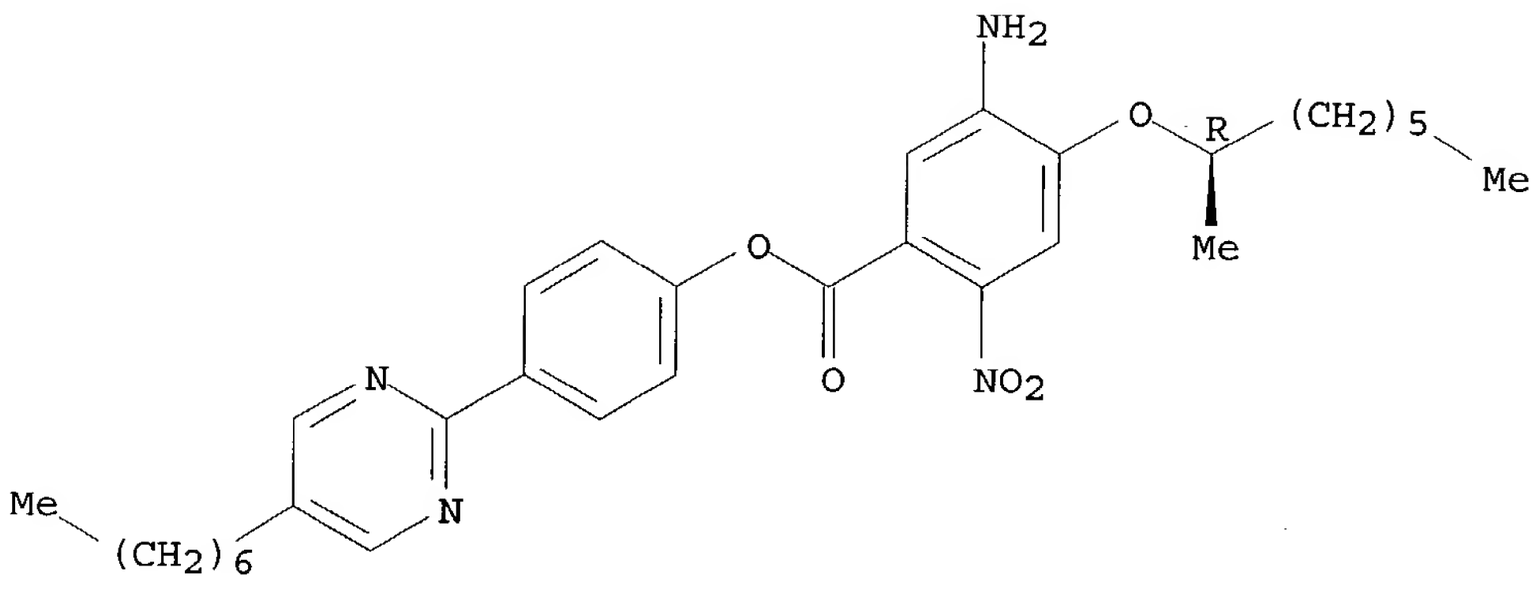
L11 ANSWER 44 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:192841 CAPLUS
DOCUMENT NUMBER: 124:290393
TITLE: The synthesis of nitroaniline monomers and polymers as non-linear optical ferroelectric liquid crystals
AUTHOR(S): Chen, X. H.; Herr, R. P.; Schmitt, K.; Buchecker, R.
CORPORATE SOURCE: Dep. RLCR, F. Hoffmann-La Roche Ltd., Basel, 4002, Switz.
SOURCE: Liquid Crystals (1996), 20(2), 125-38
CODEN: LICRE6; ISSN: 0267-8292
PUBLISHER: Taylor & Francis
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Chiral 2-amino-4-alkoxy-5-nitrobenzoate and 5-amino-4-alkoxy-2-nitrobenzoate derivs. as well as the corresponding biphenyl derivs. were synthesized. Some of them were also derivatized to the corresponding acrylates and polyacrylates. Many of the new substances exhibit a large spontaneous polarization and large second-order NLO coeffs. In addition some of them show a broad range SC* phase. All these properties depend strongly on small changes in the mol. structures. Here we present the synthesis of these novel NLO FLC materials and discuss some of their properties.

IT **147970-12-5**
RL: PRP (Properties)
(nitroaniline monomers and polymers as nonlinear optical ferroelec. liquid crystals)

RN 147970-12-5 CAPLUS
CN Benzoic acid, 5-amino-4-[(1-methylheptyl)oxy]-2-nitro-, 4-(5-heptyl-2-pyrimidinyl)phenyl ester, (R)- (9CI) (CA INDEX NAME)

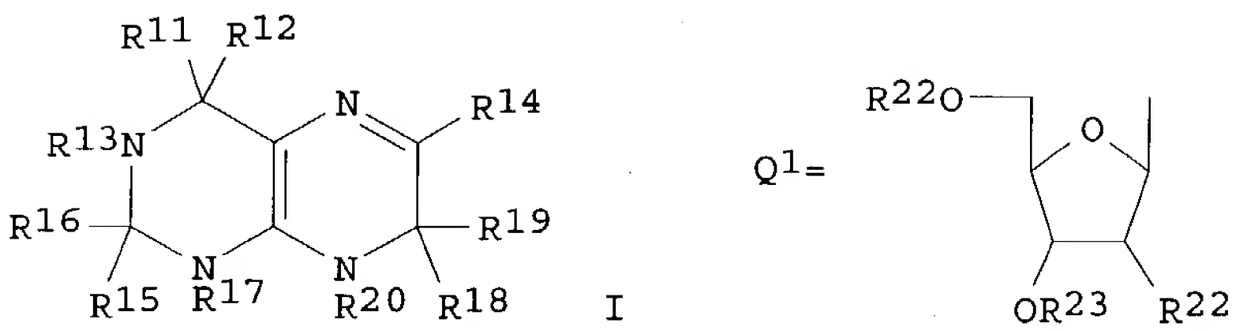
Absolute stereochemistry.




L11 ANSWER 45 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:170748 CAPLUS
DOCUMENT NUMBER: 124:261618
TITLE: Preparation of pteridine nucleotide analogs as fluorescent DNA probes.
INVENTOR(S): Hawkins, Mary E.; Pfleiderer, Wolfgang; Davis, Michael Dean; Balis, Frank
PATENT ASSIGNEE(S): United States Dept. of Health and Human Services, USA
SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9531469 | A1 | 19951123 | WO 1995-US5264 | 19950425 |
| W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT | | | | |
| RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| US 5525711 | A | 19960611 | US 1994-245923 | 19940518 |
| CA 2190588 | AA | 19951123 | CA 1995-2190588 | 19950425 |
| CA 2190588 | C | 20030318 | | |
| AU 9523991 | A1 | 19951205 | AU 1995-23991 | 19950425 |
| AU 688036 | B2 | 19980305 | | |
| EP 759927 | A1 | 19970305 | EP 1995-917197 | 19950425 |
| EP 759927 | B1 | 19980624 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE | | | | |
| JP 10500949 | T2 | 19980127 | JP 1995-529675 | 19950425 |
| AT 167680 | E | 19980715 | AT 1995-917197 | 19950425 |
| ES 2118593 | T3 | 19980916 | ES 1995-917197 | 19950425 |
| US 5612468 | A | 19970318 | US 1995-451641 | 19950526 |

PRIORITY APPLN. INFO.: US 1994-245923 A 19940518
WO 1995-US5264 W 19950425
OTHER SOURCE(S): MARPAT 124:261618
GI



I

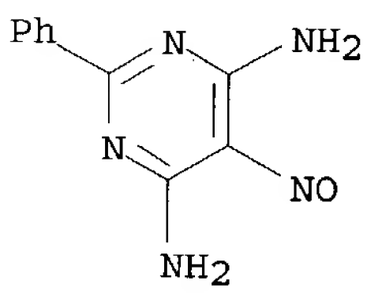


AB Title compds. [I; R11R12 = O, or R11R13 = bond; R12 = (protected) NH2; R13 = H, alkyl; R14 = H, alkyl, Ph; R15R16 = O, or R15R17 = bond; R16 = H, Ph, (protected) NH2; R18R19 = O; R18R20 = bond; R17, R20 = Q1; R21 = H, triphosphate, protecting group; R22 = H, (protected) OH; R23 = H, phosphoramidite, phosphonate, methylphosphonate, phosphorothioate, phosphotriester, hemisuccinate (bound to a solid support), carbodiimide (bound to a solid support); with provisos], were prepared Thus, 4-amino-6-**phenyl**-8-(5-O-dimethoxytrityl-2-deoxy-β-D-ribofuranosyl)pteridine-7-one 3'-O-(β-cyanoethyl, N-diisopropyl)phosphoramidite was prepared via 4-amino-6-phenylpteridine-7-one and used in a double-stranded DNA segment for realtime determination of HIV-1 integrase activity.

IT **56472-04-9P**, 2-**Phenyl**-4,6-diamino-5-nitrosopyrimidine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pteridine nucleotide analogs as fluorescent DNA probes)

RN 56472-04-9 CAPLUS

CN 4,6-Pyrimidinediamine, 5-nitroso-2-phenyl- (9CI) (CA INDEX NAME)



L11 ANSWER 46 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:137584 CAPLUS
DOCUMENT NUMBER: 124:176140
TITLE: Preparation of optically active heteroarylalkanol and arylalkanol
INVENTOR(S): Azumai, Takayuki; Minamii, Masayoshi; Fujimoto, Yukari; Matsumoto, Tsutomu
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 07291940 | A2 | 19951107 | JP 1994-89663 | 19940427 |
| JP 3486685 | B2 | 20040113 | | |

PRIORITY APPLN. INFO.: JP 1994-89663 19940427
OTHER SOURCE(S): CASREACT 124:176140; MARPAT 124:176140
GI

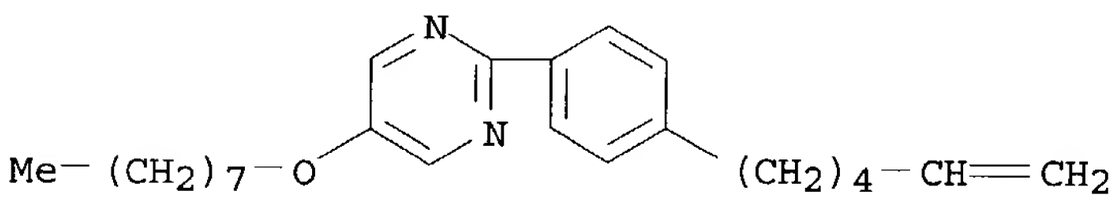
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compound represented by formula R1(O)mA1(A2)pA3(CH2)nR [I; R = CH(OH)Me; R1 = C1-20 (halo)alkyl, C2-20 (halo)alkoxyalkyl; A1, A2, A3 = Q - Q9; wherein u, w = 0-3; provided that when A1 = fused ring, A2 = monocyclic ring or when A1 = monocyclic ring and p = 1, A2 and A3 = monocyclic ring; n = 0-10; m, p = 0,1], useful as an intermediate for agrochems., drugs and ferroelec. liquid crystals, is prepared by hydrosilyation of an α-alkene I (R = CH:CH2) with HSi(X5)3 (X5 = H, alkyl, alkoxy, halo) in the presence of a transition metal complex having an optically active tert-phosphine binaphthyl compound [R2 = halo, alkoxy, alkoxyalkoxy, (**phenyl**)alkyl, C5-7 cycloalkyl; R3 = alkyl, alkoxy, (halo)**phenyl**; R4, R5 = H, alkyl; or R4R5 forms a fused ring] and oxidation of the resulting silane I [R = CHMeSi(X5)3]. Thus, 5.4 g trichlorosilane was slowly added dropwise to a mixture of 10 g 2-[4-(5-hexen-1-yl)**phenyl**]-5-octyloxypyrimidine, 0.46 mg π-allylpalladium chloride, and 1.22 mg (S)-I (R2 = Me, R3 = Ph, R4 = R5 = H) at 25-30° and the resulting mixture was stirred for 10 h and added to a suspension of 1.7 g KF and 9 g KHCO3 in 100 mL THF and 100 mL MeOH under ice-cooling. The resulting mixture was stirred under ice-cooling for 2 h, followed by adding 25 mL 30% H2O2, and the reaction mixture was stirred at 50° for 24 h to give, after silica gel chromatog., the optically active title compound [(-)-II].

IT **165320-52-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of optically active heteroarylalkanol and arylalkanol by hydrosilylation of heteroaryl- or aryl-α-alkene with trichlorosilane)

RN 165320-52-5 CAPLUS

CN Pyrimidine, 2-[4-(5-hexenyl)phenyl]-5-(octyloxy)- (9CI) (CA INDEX NAME)




L11 ANSWER 47 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:950790 CAPLUS
DOCUMENT NUMBER: 124:144907
TITLE: An efficient procedure for palladium-catalyzed reduction of aryl/enol triflates
AUTHOR(S): Kotsuki, Hiyoshizo; Datta, Probal Kanti; Hayakawa, Hiroyuki; Suenaga, Hitoshi
CORPORATE SOURCE: Dep. of Chemistry, Kochi Univ., Kochi, 780, Japan
SOURCE: Synthesis (1995), (11), 1348-50
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:144907

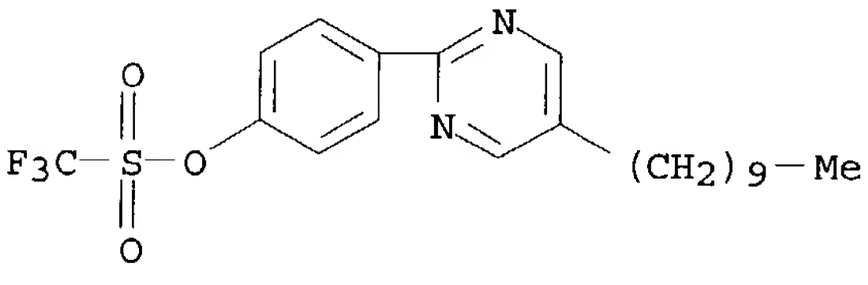
AB An efficient procedure to deoxygenate phenols and enols via trifluoromethanesulfonates is presented. Their reduction with Et3SiH in the presence of a catalytic amount of Pd(OAc)2 and bidentate phosphine ligands such as 1,3-bis(diphenylphosphino)propane or 1,1'-bis(diphenylphosphino)ferrocene proceeded efficiently to afford a variety

of aromatic, heteroarom., and olefinic compds.

IT **173346-92-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(palladium-catalyzed reduction of aryl enol triflates with triethylsilane)

RN 173346-92-4 CAPLUS

CN Methanesulfonic acid, trifluoro-, 4-(5-decyl-2-pyrimidinyl)phenyl ester (9CI) (CA INDEX NAME)

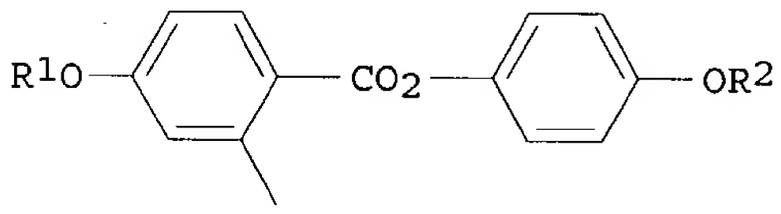


L11 ANSWER 48 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:604529 CAPLUS
DOCUMENT NUMBER: 123:156562
TITLE: **Phenyl** ester compound, its manufacture, and ferroelectric liquid-crystal mixture containing the compound
INVENTOR(S): Ishizuka, Hidemi; Nishama, Isa; Yokoyama, Akihisa
PATENT ASSIGNEE(S): Japan Enajii Kk, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 07089904 | A2 | 19950404 | JP 1993-233272 | 19930920 |

PRIORITY APPLN. INFO.: JP 1993-233272 19930920
OTHER SOURCE(S): MARPAT 123:156562
GI



II

AB The Ph ester is QOCOCH2CHMe(CH2)2CO2Q (I; R1-2 = C1-15 alkyl). I may be optically active QOCOCH2C*HMe(CH2)2CO2Q (Q=II). The mixture contains ≥1 I. I is manufactured by esterification of 2 equivalent 5-alkyloxy-2-(4-alkyloxyphenoxycarbonyl)phenol QOH and 1 equivalent XOC(CH2)2CHMeCH2COX (X = OH, halo). The compound is useful to control cholesteric pitches of ferroelec. liquid-crystal mixts. for electrooptical elements.

IT **166522-78-7**
RL: TEM (Technical or engineered material use); USES (Uses)
(ferroelec. liquid-crystal mixture containing optically active Ph ester)

RN 166522-78-7 CAPLUS

CN Hexanedioic acid, 3-methyl-, bis[5-(octyloxy)-2-[[4-(octyloxy)phenoxy]carbonyl]phenyl] ester, (R)-, mixt. with 2-[4-(decyloxy)phenyl]-5-octylpyrimidine, 2-[4-(hexyloxy)phenyl]-5-

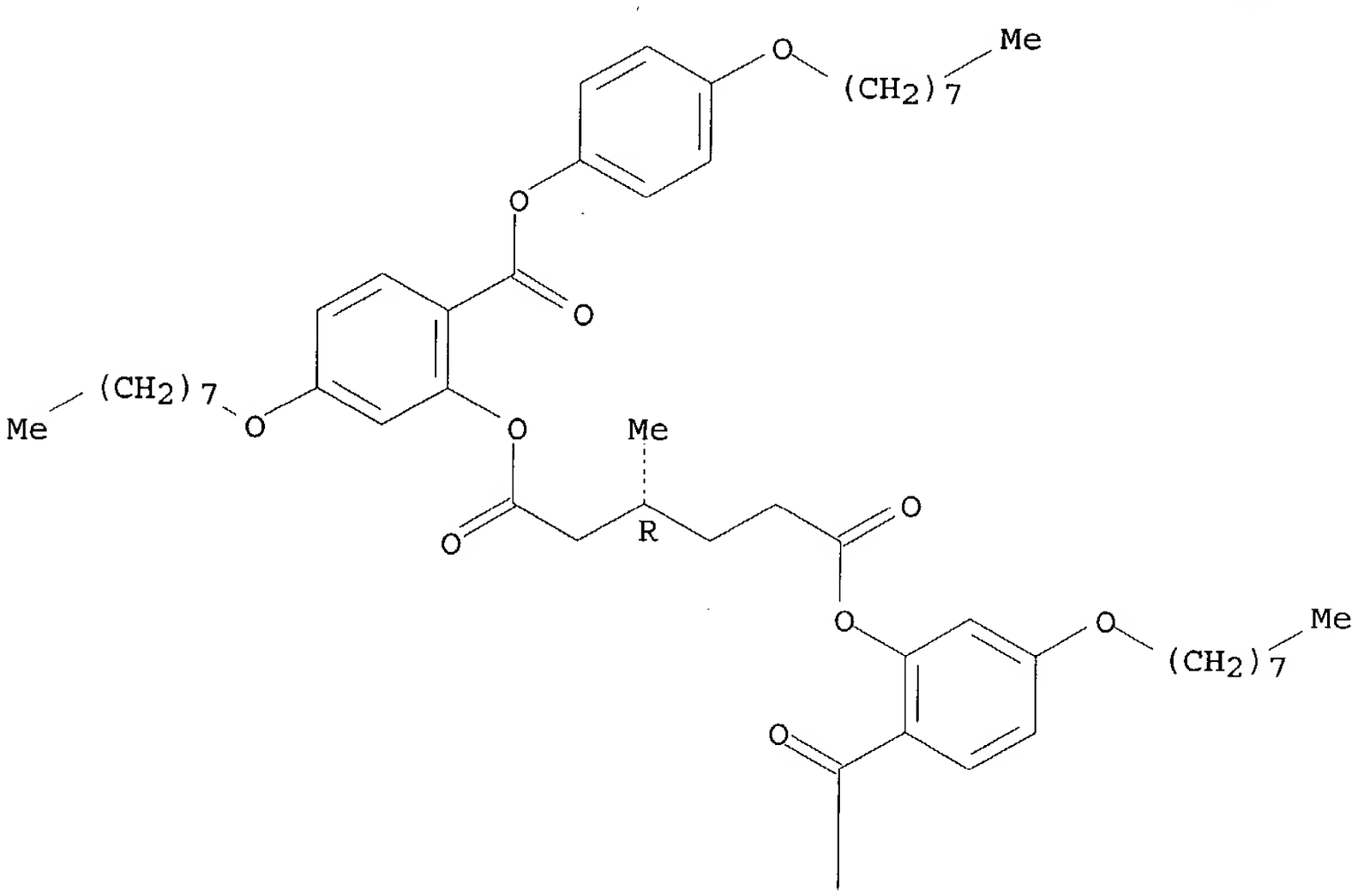
nonylpyrimidine, 2-[4-(hexyloxy)phenyl]-5-octylpyrimidine and 2-[4-(nonyloxy)phenyl]-5-octylpyrimidine (9CI) (CA INDEX NAME)

CM 1

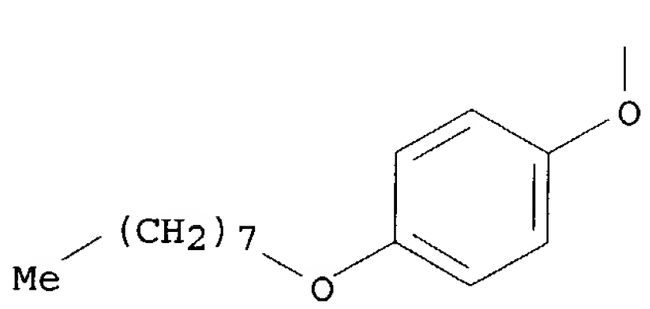
CRN 165686-74-8
CMF C65 H92 O12

Absolute stereochemistry.

PAGE 1-A

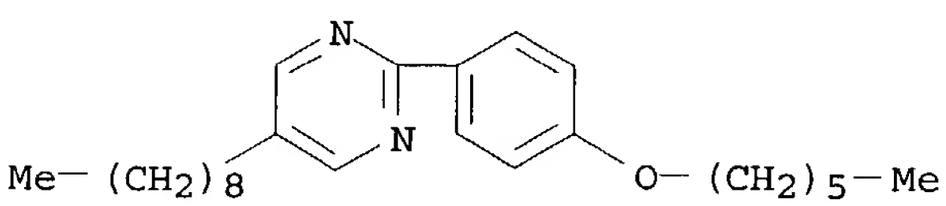



PAGE 2-A



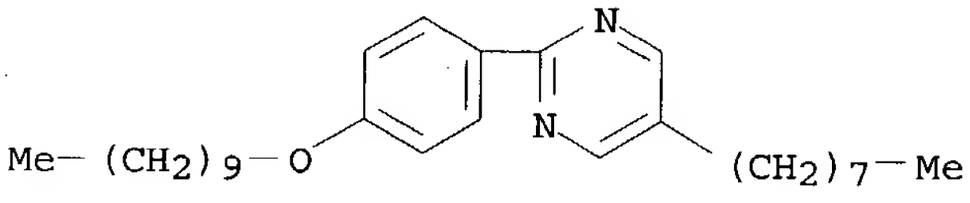

CM 2

CRN 57202-56-9
CMF C25 H38 N2 O



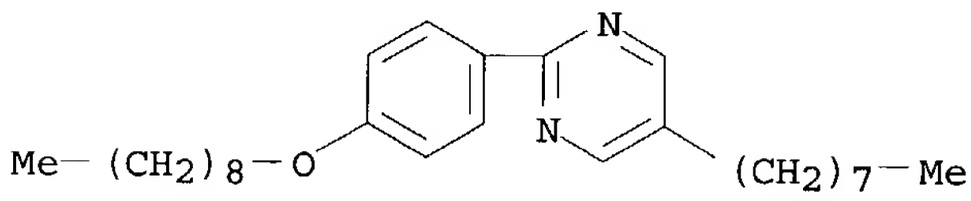
CM 3

CRN 57202-52-5
CMF C28 H44 N2 O



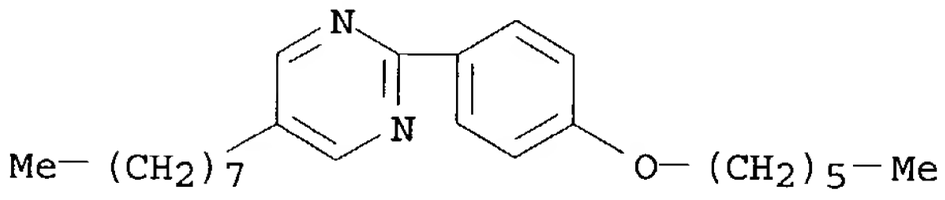
CM 4

CRN 57202-51-4
CMF C27 H42 N2 O



CM 5

CRN 57202-48-9
CMF C24 H36 N2 O

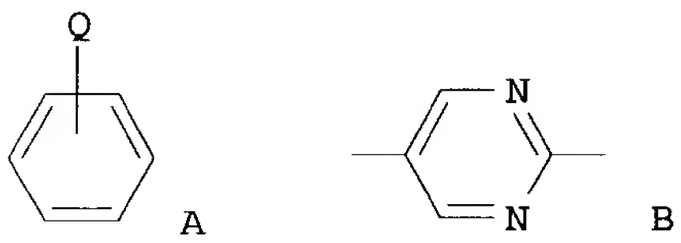


L11 ANSWER 49 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:576985 CAPLUS
DOCUMENT NUMBER: 123:98128
TITLE: **Phenyl** benzoate derivative optically active compound, liquid-crystal composition containing it, and phenolic derivative intermediate
INVENTOR(S): Kobayashi, Shogo; Ishibashi, Shigeki; Horie, Toshio; Tsuru, Shinji; Nakamura, Kozaburo; Maruno, Tooru
PATENT ASSIGNEE(S): Nippon Telegraph & Telephone, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 07069990 | A2 | 19950314 | JP 1994-136138 | 19940617 |
| JP 07121892 | B4 | 19951225 | | |

09/ 811,359

PRIORITY APPLN. INFO.: JP 1994-136138 19940617
OTHER SOURCE(S): MARPAT 123:98128
GI




A B

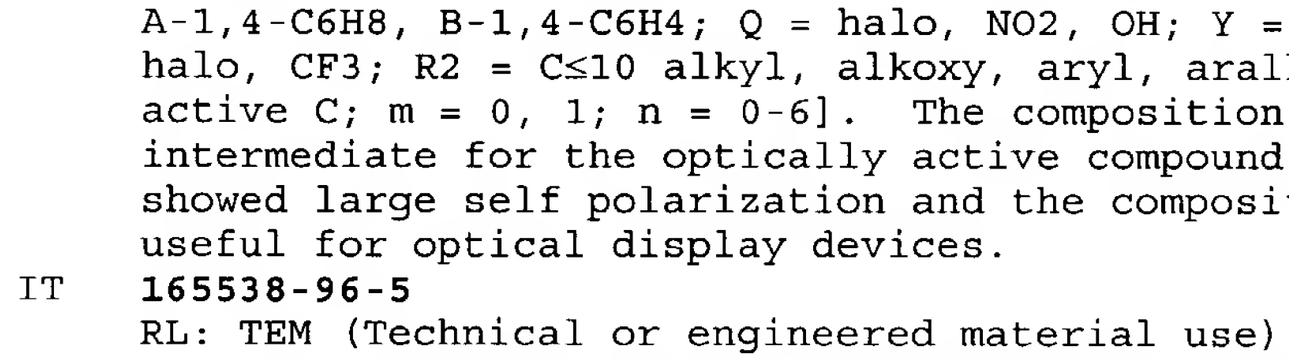
AB The compound is a Ph benzoate derivative I [W = R1XCO2; R1 = C4-22 alkyl, C4-22 alkoxy; X = 1,4-C6H4, A, (1,4-C6H4)2, A-1,4-C6H4, 1,4-C6H4-1,4-C6H8, A-1,4-C6H8, B-1,4-C6H4; Q = halo, NO2, OH; Y = halo, Me, NO2; Z = Me, halo, CF3; R2 = C≤10 alkyl, alkoxy, aryl, aralkyl; C* = optically active C; m = 0, 1; n = 0-6]. The composition contains ≥1 I. The intermediate for the optically active compound is I (W = OH). The compound showed large self polarization and the composition showed high response to be useful for optical display devices.

IT **165538-96-5**
RL: TEM (Technical or engineered material use); USES (Uses)
(Ph benzoate derivative optically active compound and ferroelec. liquid-crystal composition containing it and its intermediate)

RN 165538-96-5 CAPLUS
CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-(octyloxy)-, 3-methyl-4-(2-methyl-1-oxobutyl)phenyl ester, mixt. with 5-(heptyloxy)-2-[4-(nonyloxy)phenyl]pyrimidine, 2-[4-(hexyloxy)phenyl]-5-(octyloxy)pyrimidine and 5-(octyloxy)-2-[4-(octyloxy)phenyl]pyrimidine (9CI) (CA INDEX NAME)

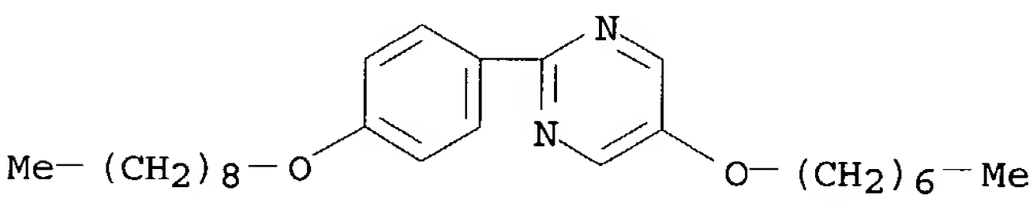
CM 1

CRN 123020-69-9
CMF C33 H40 O4



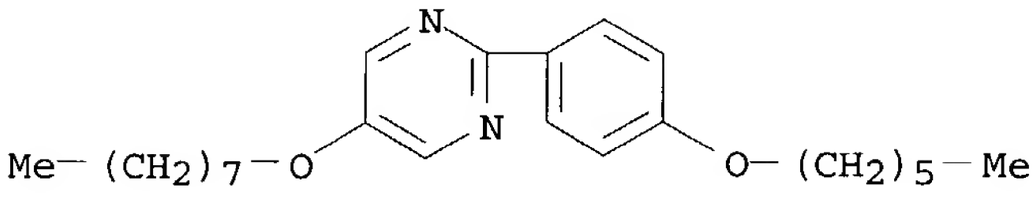

CM 2

CRN 121554-50-5
CMF C26 H40 N2 O2



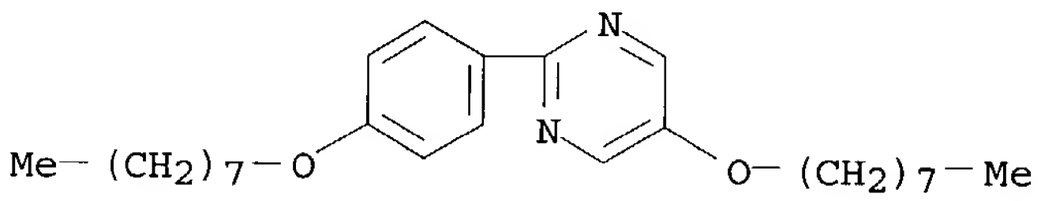
CM 3

CRN 120091-49-8
CMF C24 H36 N2 O2



CM 4

CRN 114767-84-9
CMF C26 H40 N2 O2



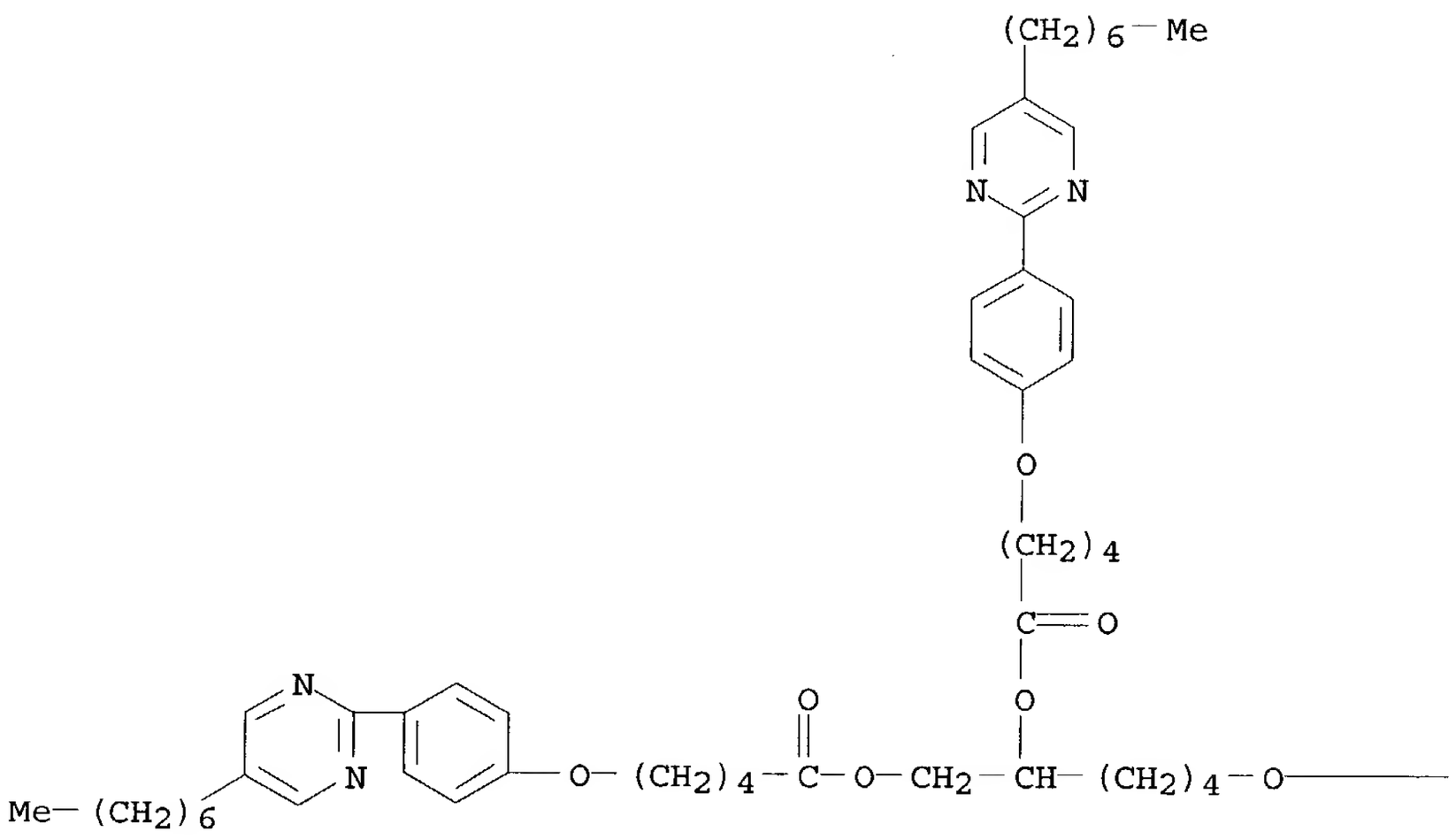
L11 ANSWER 50 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:513318 CAPLUS
DOCUMENT NUMBER: 123:71030
TITLE: Heterotrimeric liquid crystalline thiadiazole derivatives
AUTHOR(S): Zab, Kerstin; Joachimi, Detlev; Novotna, Eva; Diele, Siegmar; Tschierske, Carsten
CORPORATE SOURCE: Dep. Chem., Martin-Luther-Univ., Saale, Weinbergweg, D-06015/16, Germany
SOURCE: Liquid Crystals (1995), 18(4), 631-7
CODEN: LICRE6; ISSN: 0267-8292
PUBLISHER: Taylor & Francis
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Various trimeric cooligomers combining 2-**phenyl**-1,3,4-thiadiazole mesogenic moieties with a biphenyl mesogenic moiety were synthesized and their mesomorphic behavior studied by polarizing microscopy, calorimetry and x-ray scattering. Such cooligomeric structures provide an opportunity to combine different mesogenic units. Thus readily accessible homochiral biphenyl mesogenic units were connected with thiadiazole mesogenic units leading to an oligomeric liquid crystal material with ferroelec. properties.

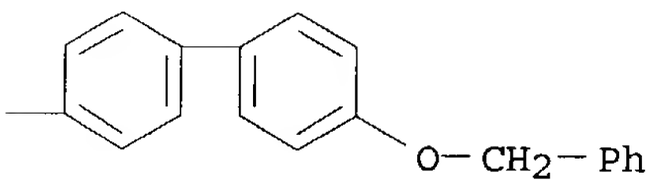
IT **164667-82-7P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation and ferroelec. and liquid crystal properties of)

RN 164667-82-7 CAPLUS
CN Pentanoic acid, 5-[4-(5-heptyl-2-pyrimidinyl)phenoxy]-, 1-[4-[[4'-(phenylmethoxy)[1,1'-biphenyl]-4-yl]oxy]butyl]-1,2-ethanediyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L11 ANSWER 51 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:489324 CAPLUS
DOCUMENT NUMBER: 123:22735
TITLE: Trimeric and tetrameric liquid crystalline thiadiazole derivatives
AUTHOR(S): Zab, K.; Joachimi, D.; Agert, O.; Neumann, B.; Tschierske, C.
CORPORATE SOURCE: Inst. Org. Chem., Martin-Luther-Univ.

Halle-Wittenberg, Halle/Saale, D-06015, Germany
SOURCE: Liquid Crystals (1995), 18(3), 489-94
CODEN: LICRE6; ISSN: 0267-8292
PUBLISHER: Taylor & Francis
DOCUMENT TYPE: Journal
LANGUAGE: English

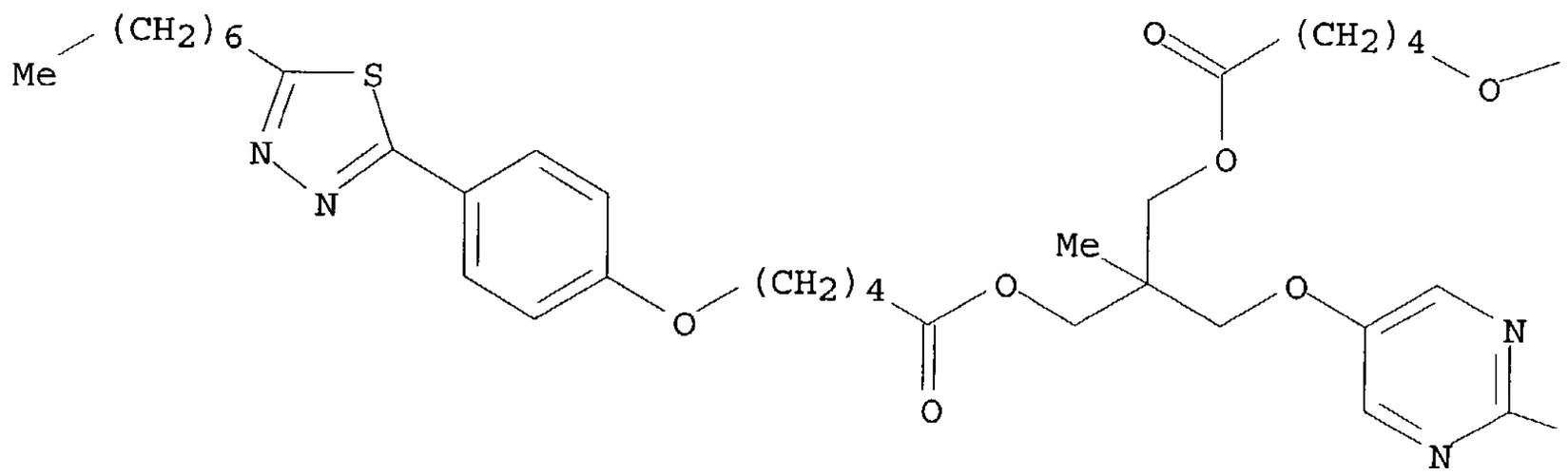
AB Novel liquid crystalline 2-**phenyl**-1,3,4-thiadiazole based oligomers with three and four rigid aromatic units linked by a flexible central unit were studied by polarizing microscopy. The synthesis of these compds. and the influence of structural variations on the mesomorphic properties are described. The combination of suitable mesogenic moieties with appropriate central units leads to oligomers which exhibit SC phases.

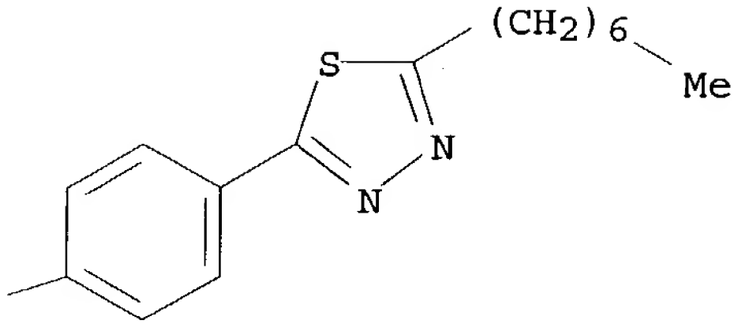
IT **164074-96-8P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(preparation and liquid crystals properties of)

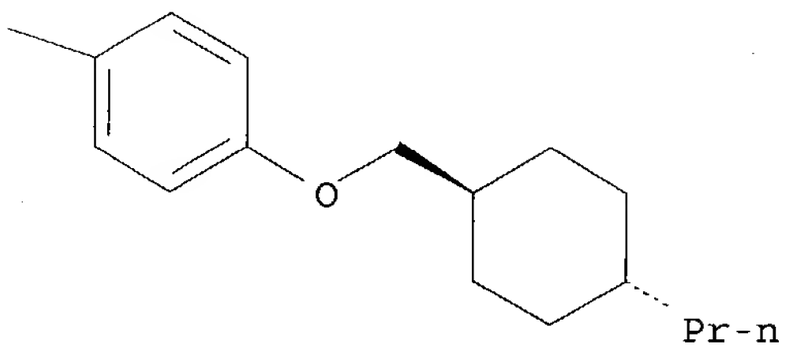
RN 164074-96-8 CAPLUS
CN Pentanoic acid, 5-[4-(5-heptyl-1,3,4-thiadiazol-2-yl)phenoxy]-, 2-methyl-2-[[[2-[4-[(4-propylcyclohexyl)methoxy]phenyl]-5-pyrimidinyl]oxy]methyl]-1,3-propanediyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.








L11 ANSWER 52 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:207982 CAPLUS
DOCUMENT NUMBER: 122:93024
TITLE: Perfluoroalkyloxyphenyl fluoroalkyloxybenzoate, its preparation, its-containing liquid crystal composition, and display
INVENTOR(S): Nohira, Hiroyuki; Sakaigawa, Akira
PATENT ASSIGNEE(S): Idemitsu Petrochemical Co, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 06239802 | A2 | 19940830 | JP 1993-46113 | 19930212 |

PRIORITY APPLN. INFO.: JP 1993-46113 19930212
OTHER SOURCE(S): MARPAT 122:93024

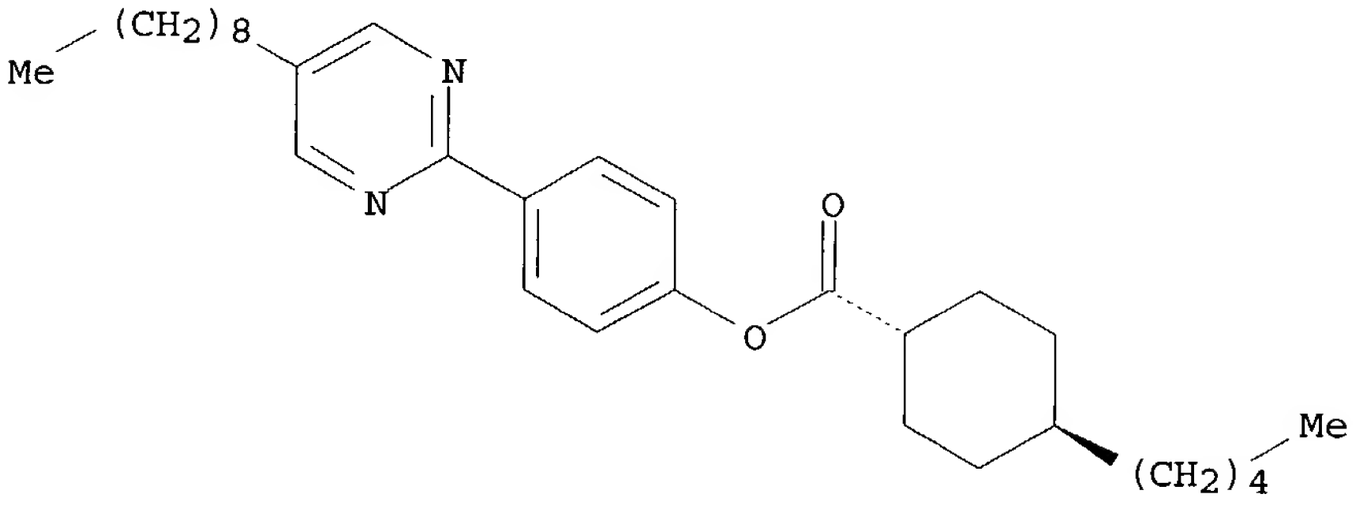
AB The title compound consists of CmH2m+1CHFCH2O-1,4-C6H4CO2-1,4-C6H4OCH2CnF2n+1 (I; m, n = 1-20) or I (m = 6, n = 7). The compound is prepared by esterification of HO-1,4-C6H4OCH2CnF2n+1 and CmH2m+1CHFCH2O-1,4-C6H4CO2H. The liquid crystal composition contains smectic liquid crystal compds. and the claimed compound The display is obtained by using the composition The compound showed high spontaneous polarization and rapid response.

IT **160189-32-2**
RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)
(liquid crystal display containing perfluoroalkyloxyphenyl fluoroalkyloxybenzoate with high spontaneous polarization and rapid response)

RN 160189-32-2 CAPLUS
CN Cyclohexanecarboxylic acid, 4-pentyl-, 4-(5-nonyl-2-pyrimidinyl)phenyl

ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

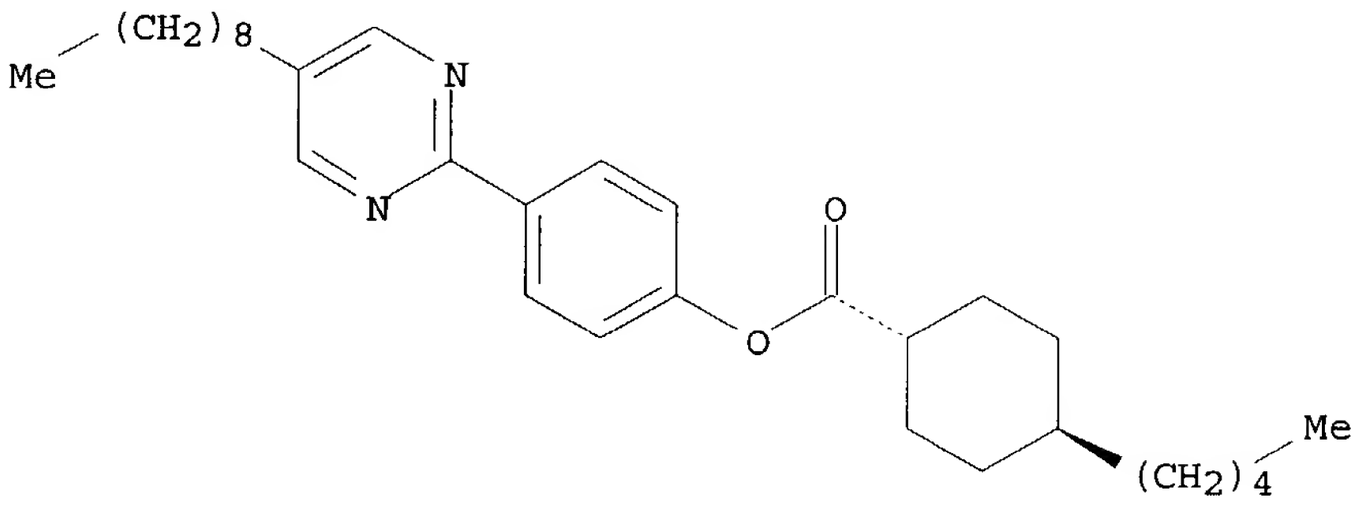


L11 ANSWER 53 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:207981 CAPLUS
DOCUMENT NUMBER: 122:93023
TITLE: Perfluoroalkyloxyphenyl fluoroalkylbenzoate, its preparation, its-containing liquid crystal composition, and display
INVENTOR(S): Nohira, Hiroyuki; Sakaigawa, Akira; Imamura, Shinichi
PATENT ASSIGNEE(S): Idemitsu Petrochemical Co, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 06239800 | A2 | 19940830 | JP 1993-46114 | 19930212 |

PRIORITY APPLN. INFO.: JP 1993-46114 19930212
OTHER SOURCE(S): MARPAT 122:93023
AB The title compound consists of CmH2m+1C(CF3)H-1,4-C6H4CO2-1,4-C6H4OCH2CnF2n+1 (I; m, n = 1-20) or I (m = 6, n = 7). The compound is prepared by esterification of HO-1,4-C6H4OCH2CnF2n+1 and CmH2m+1C(CF3)H-1,4-C6H4CO2H. The liquid crystal composition contains smectic liquid crystal compds. and the claimed compound The display is obtained by using the composition The compound showed high spontaneous polarization and rapid response.
IT **160189-32-2**
RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)
(liquid crystal display containing perfluoroalkyloxyphenyl fluoroalkylbenzoate with high spontaneous polarization and rapid response)
RN 160189-32-2 CAPLUS
CN Cyclohexanecarboxylic acid, 4-pentyl-, 4-(5-nonyl-2-pyrimidinyl)phenyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



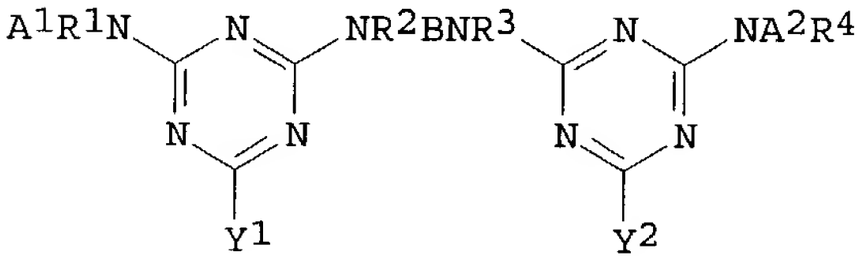
L11 ANSWER 54 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:485637 CAPLUS
DOCUMENT NUMBER: 121:85637
TITLE: Dyeing of cellulose-containing fiber materials with reactive dyes
INVENTOR(S): Landre, Jean Francois; Tzikas, Athanassios; Luttringer, Jean Pierre
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

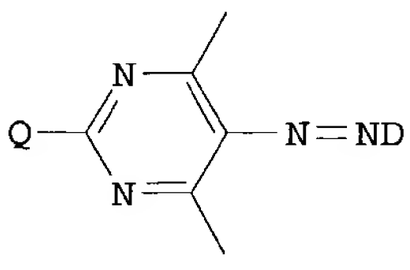
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9318224 | A1 | 19930916 | WO 1993-EP426 | 19930224 |
| W: AU, BB, BG, BR, CA, CZ, FI, HU, JP, KP, KR, KZ, LK, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG | | | | |
| AU 9336297 | A1 | 19931005 | AU 1993-36297 | 19930224 |
| AU 677575 | B2 | 19970501 | | |
| EP 629249 | A1 | 19941221 | EP 1993-905272 | 19930224 |
| EP 629249 | B1 | 19970108 | | |
| R: BE, CH, DE, DK, ES, FR, GB, IT, LI, PT | | | | |
| JP 07504949 | T2 | 19950601 | JP 1993-515289 | 19930224 |
| ES 2098727 | T3 | 19970501 | ES 1993-905272 | 19930224 |
| BR 9306026 | A | 19971118 | BR 1993-6026 | 19930224 |
| CA 2129750 | C | 20030506 | CA 1993-2129750 | 19930224 |
| US 5525124 | A | 19960611 | US 1994-295765 | 19940902 |

| | | | |
|---|---|---|---|
| PRIORITY APPLN. INFO.: | CH 1992-714 | A | 19920306 |
| | CH 1992-715 | A | 19920306 |
| | WO 1993-EP426 | A | 19930224 |

OTHER SOURCE(S): MARPAT 121:85637
GI



I



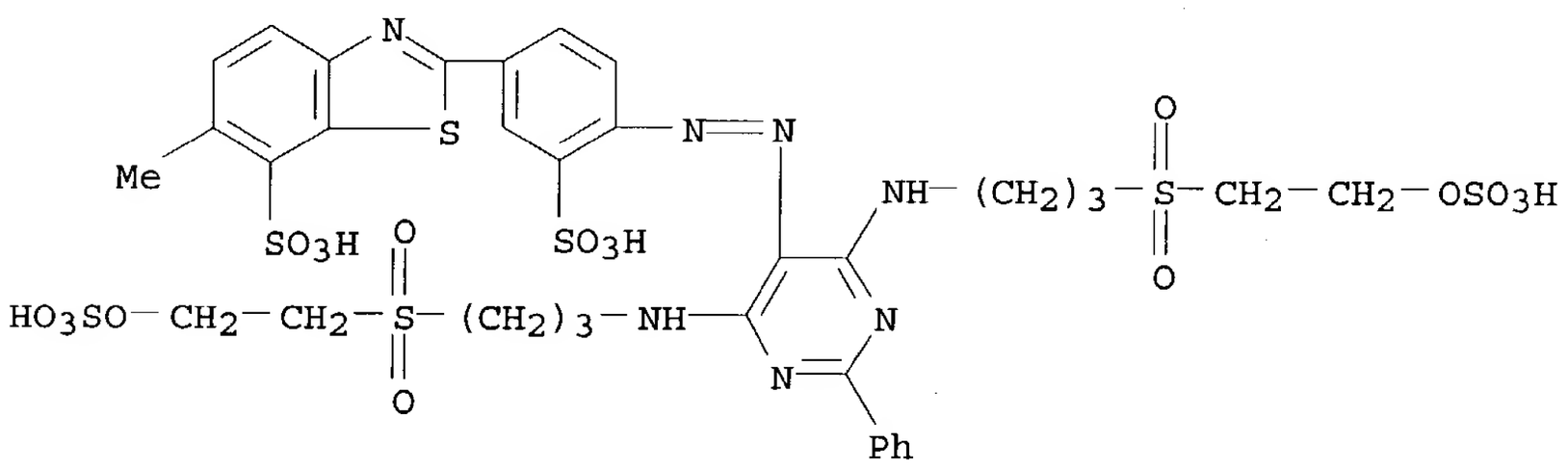
II

AB Title process comprises dyeing in a dyebath containing 0-20 g/L mineral acid salt, e.g., NaCl or Na2SO4, and ≥1 reactive dye (I) (A1 = dye chromophore, A2 = A1, H, colorless organic residue; R1-4 = H, unsubstituted C1-4 alkyl; B = aliphatic or aromatic bridging group; Y1, Y2 = F, carboxypyridinium) and (II) (Q = optionally substituted Ph, **naphthyl**, heteroaryl; D = diazo radical; R5, R6 = optionally substituted amino, ≥1 R5, R6, or D contains a fiber-reactive group). The process produces dyeings with good fastness and high color yields without the addition of large amts. of mineral acid salts.

IT **156202-64-1**
RL: USES (Uses)
(dyeing of cotton by, in presence of low amts. of mineral acid salts)

RN 156202-64-1 CAPLUS

CN 7-Benzothiazolesulfonic acid, 6-methyl-2-[4-[[2-phenyl-4,6-bis[[3-[[2-(sulfooxy)ethyl]sulfonyl]propyl]amino]-5-pyrimidinyl]azo]-3-sulfophenyl]- (9CI) (CA INDEX NAME)



L11 ANSWER 55 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:408893 CAPLUS

DOCUMENT NUMBER: 121:8893

TITLE: **Phenyl**-substituted acrylate ester agrochemical fungicides

INVENTOR(S): Mueller, Bernd; Roehl, Franz; Koenig, Hartmann; Sauter, Hubert; Lorenz, Gisela; Ammermann, Eberhard

PATENT ASSIGNEE(S): BASF A.-G., Germany

SOURCE: Eur. Pat. Appl., 86 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

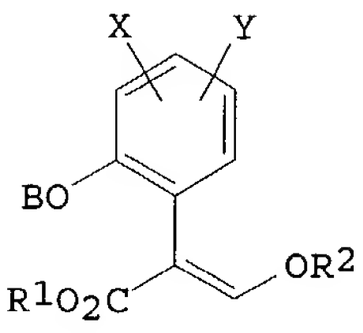
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 581095 | A2 | 19940202 | EP 1993-111103 | 19930712 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, NL, PT, SE | | | | |
| CA 2100546 | AA | 19940125 | CA 1993-2100546 | 19930714 |
| JP 06211748 | A2 | 19940802 | JP 1993-181305 | 19930722 |
| AU 9342121 | A1 | 19940127 | AU 1993-42121 | 19930723 |
| AU 660226 | B2 | 19950615 | | |
| HU 66105 | A2 | 19940928 | HU 1993-2150 | 19930723 |
| ZA 9305332 | A | 19950123 | ZA 1993-5332 | 19930723 |

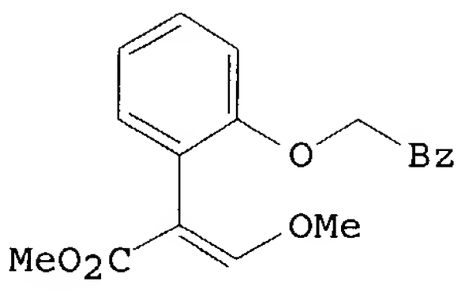
PRIORITY APPLN. INFO.: DE 1992-4224457 19920724

OTHER SOURCE(S): MARPAT 121:8893

GI




I




II

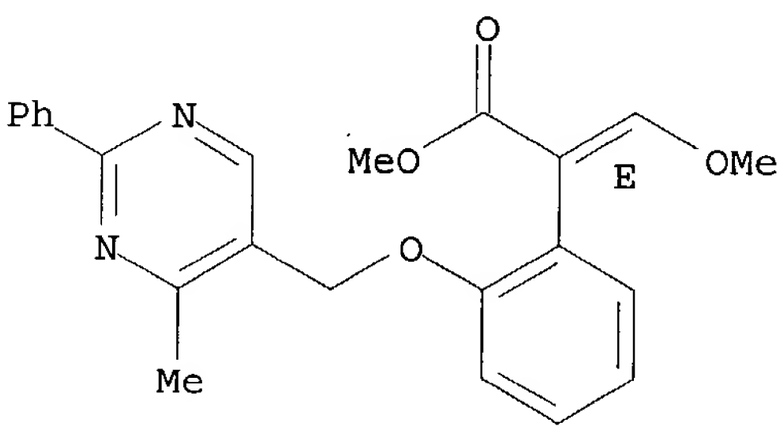
AB The title compds. [I; B = (un)substituted alkyl, C1-4 (un)substituted alkenyl, (un)substituted alkynyl, etc.; R1, R2 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, etc.; X, Y = H, halogen, CN, NO2, haloalkyl, alkyl, alkenyl, alkynyl, heteroaryl, heterocyclyl, etc.], useful as agrochem. fungicides, are prepared and I-containing formulations presented. Thus, Me α-(2-hydroxyphenyl)-β-methoxyacrylate was condensed with phenacyl bromide, producing acrylate II, m.p. 76°, which demonstrated 90% inhibitory activity against Plasmopara viticola at 250 ppm.

IT **154594-91-9P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as agrochem. fungicide)

RN 154594-91-9 CAPLUS

CN Benzeneacetic acid, α-(methoxymethylene)-2-[(4-methyl-2-phenyl-5-pyrimidinyl)methoxy]-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



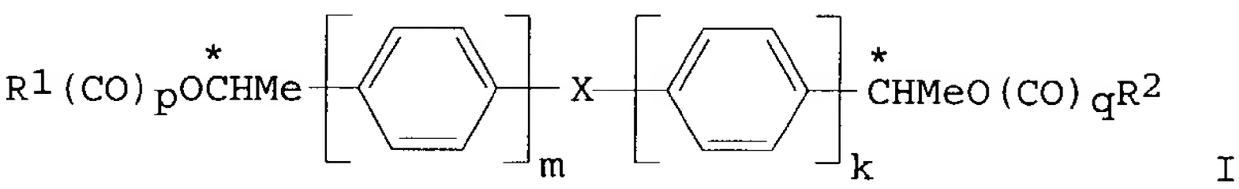

L11 ANSWER 56 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:614448 CAPLUS
DOCUMENT NUMBER: 119:214448
TITLE: Preparation of optically active aromatic esters and liquid crystal compositions containing them
INVENTOR(S): Azumai, Takayuki; Toda, Shoji; Minamii, Masayoshi
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 04337384 | A2 | 19921125 | JP 1991-110116 | 19910515 |
| JP 2906729 | B2 | 19990621 | | |

PRIORITY APPLN. INFO.: JP 1991-110116 19910515

09/ 811,359

OTHER SOURCE(S): MARPAT 119:214448
GI



I

AB The title compds. I (X = CO2, O2C; R1, R2 = halo, C1-20 alkyl, C2-20 alkoxy; m, k, l = 1, 2; p, q = 0, 1; C* denotes an asym. C atom) are prepared Liquid crystal compns. contain I for use in liquid-crystal display devices. When I are mixed to form chiral smectic C liquid crystal compns., I induce sufficient spontaneous polarization, improve orientation, and provide ferroelec. liquid crystal materials. A total of 6 optically active Ph benzoates were prepared

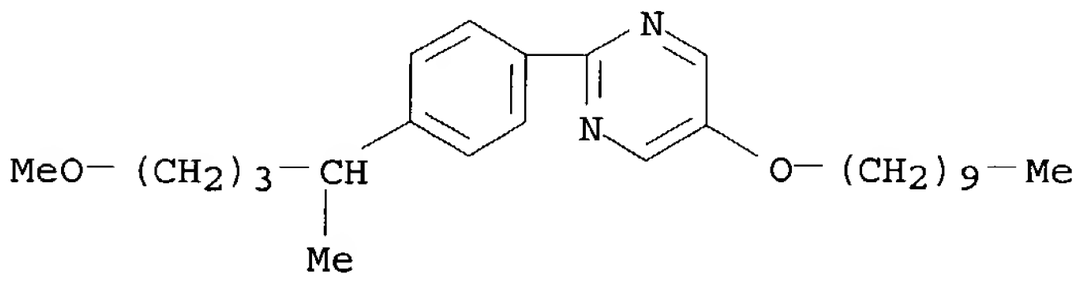
IT **150742-81-7**
RL: PRP (Properties)
(liquid crystal composition, for display)

RN 150742-81-7 CAPLUS

CN Pyrimidine, 5-(decyloxy)-2-[4-(4-methoxy-1-methylbutyl)phenyl]-, mixt. with 5-(decyloxy)-2-[4-(5-methoxypentyl)phenyl]pyrimidine (9CI) (CA INDEX NAME)

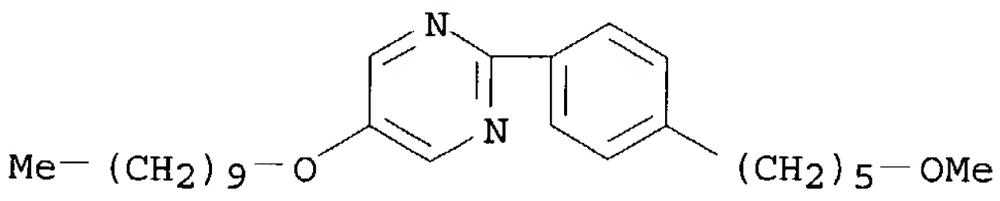
CM 1

CRN 150742-80-6
CMF C26 H40 N2 O2



CM 2

CRN 150742-79-3
CMF C26 H40 N2 O2

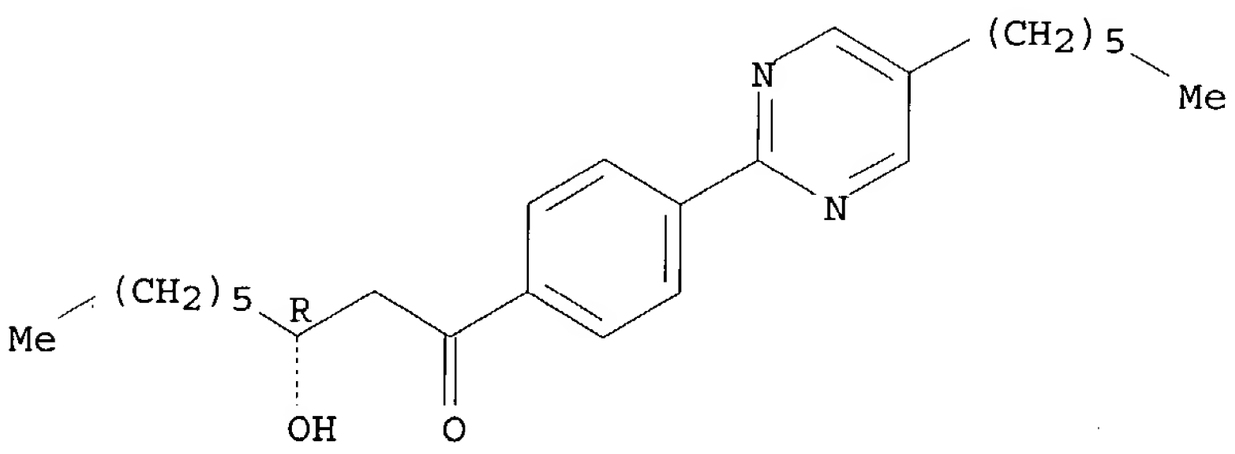


L11 ANSWER 57 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:614343 CAPLUS
DOCUMENT NUMBER: 119:214343
TITLE: Synthesis and properties of optically active 1,3-diols and their derivatives as chiral dopants for ferroelectric liquid crystals
AUTHOR(S): Kusumoto, Tetsuo; Sato, Kenichi; Ogino, Kumiko; Hiyama, Tamejiro; Takehara, Sadao; Osawa, Masashi;

09/ 811,359

Nakamura, Kayoko
CORPORATE SOURCE: Sagami Chem. Res. Cent., Sagamihara, 229, Japan
SOURCE: Liquid Crystals (1993), 14(3), 727-32
CODEN: LICRE6; ISSN: 0267-8292
DOCUMENT TYPE: Journal
LANGUAGE: English
AB New chiral dopants β-hydroxy ketones (I), 1,3-diols (II), 1,3-dioxanes (III) and 1,3-dioxan-2-ones (IV) were designed and synthesized. Reaction of (R)-1,2-epoxyoctane with carbanions derived from 2-(4-substituted **phenyl**)-1,3-dithianes followed by hydrolysis of the resulting hydroxy dithianes afforded I. Reduction of I gave the diols II, which yielded III upon acetalization and IV upon carbonation. The syn isomers of II, III, and IV exhibited larger spontaneous polarizations, when applied as chiral dopants, than the anti isomers or hydroxy ketones I.
IT **145747-60-0**
RL: PRP (Properties)
(as chiral dopant for ferroelec. liquid crystals, synthesis and properties of)
RN 145747-60-0 CAPLUS
CN 1-Nonanone, 1-[4-(5-hexyl-2-pyrimidinyl)phenyl]-3-hydroxy-, (R)- (9CI) (CA INDEX NAME)

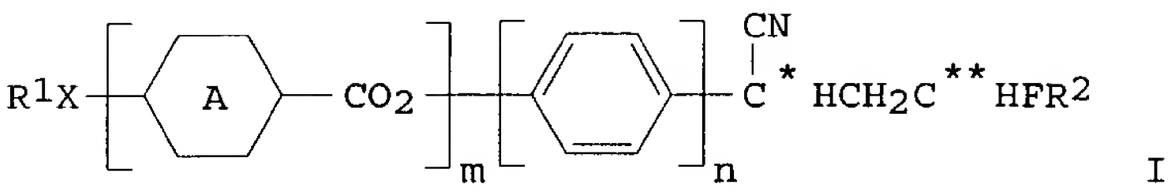
Absolute stereochemistry.



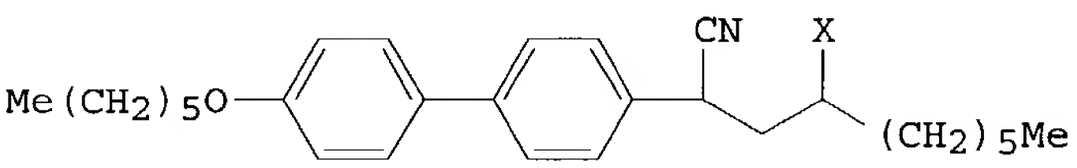

L11 ANSWER 58 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:254557 CAPLUS
DOCUMENT NUMBER: 118:254557
TITLE: Preparation of 2-**phenyl**-4-fluoroalkanenitrile derivatives, liquid crystal compositions containing them, and liquid crystal display devices
INVENTOR(S): Takehara, Sadao; Osawa, Masashi; Nakamura, Kayoko; Hiyama, Tamejiro; Kusumoto, Tetsuo; Nakayama, Akiko; Nishide, Kyoji
PATENT ASSIGNEE(S): Dainippon Ink and Chemicals, Inc., Japan; Sagami Chemical Research Center
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 04327567 | A2 | 19921117 | JP 1991-125448 | 19910426 |

PRIORITY APPLN. INFO.: JP 1991-125448 19910426
OTHER SOURCE(S): MARPAT 118:254557
GI



I



II

AB The title compds. [I; R1, R2 = C1-18 alkyl; X = O, CO2, single bond; ring A = (un)substituted 1,4-phenylene, trans-cyclohexylene; C*, C** = asym. C atoms independently having (R) or (S) configuration; m = 0, 1; n = 1, 2] are prepared When a small amount of I is added as a chiral dopant to a mother liquid crystal having smectic C phase, it induces a large spontaneous polarization and provides a ferroelec. chiral smectic liquid crystal composition with high response speed over a broad temperature range, good orientation property, and chemical stability towards H2O and light, which make it useful as a material for optical switching display devices. Thus, lithiation of 4-(4-n-hexyloxyphenyl)phenylacetonitrile with BuLi in HMPA-hexane-THF at -78° followed by addition to 1,2-epoxyoctane with warming to room temperature over 3 h gave biphenylylhydroxydecanenitrile derivative 45% (2S,4R)-II (X = OH) of 93% e.e. and 30% (2R,4R)-isomer of 93% e.e. which were fluorinated with Et2NSF3 in CH2Cl2 at -78° to 0° for 3 h to give 86% (2S,4S)-II (X = F) of 97% e.e. and 66% (2R,4R)-II (X = F) (III) of 98% e.e., resp. A liquid crystal composition containing 10% III and 90% of a mixture of 4-phenylpyrimidine derivs. showed chiral smectic C to smectic A transition at 58°, tilt angle 18.8°, spontaneous polarization +7.0 nC/cm2, and electrooptical response speed 88 μs.

IT **147553-34-2**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ferroelec. liquid crystal composition, for display)

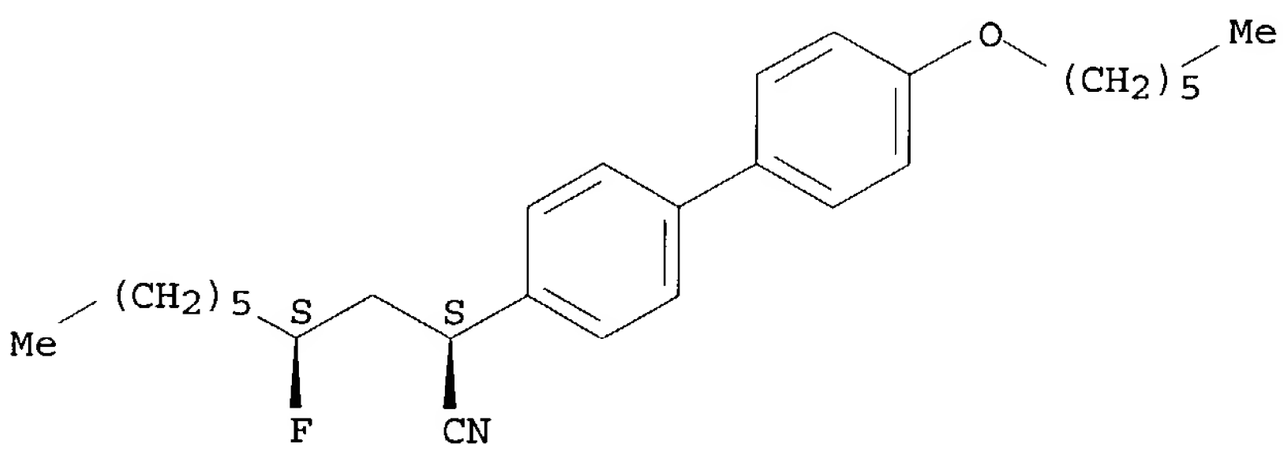
RN 147553-34-2 CAPLUS

CN [1,1'-Biphenyl]-4-acetonitrile, α-(2-fluorooctyl)-4'-(hexyloxy)-, [S-(R*,R*)]-, mixt. with 2-[4-(decyloxy)phenyl]-5-octylpyrimidine, 2-[2-fluoro-4-(octyloxy)phenyl]-5-(4-heptylphenyl)pyrimidine, 2-[4-(nonyloxy)phenyl]-5-octylpyrimidine and 5-octyl-2-[4-(octyloxy)phenyl]pyrimidine (9CI) (CA INDEX NAME)

CM 1

CRN 147224-04-2
CMF C28 H38 F N O

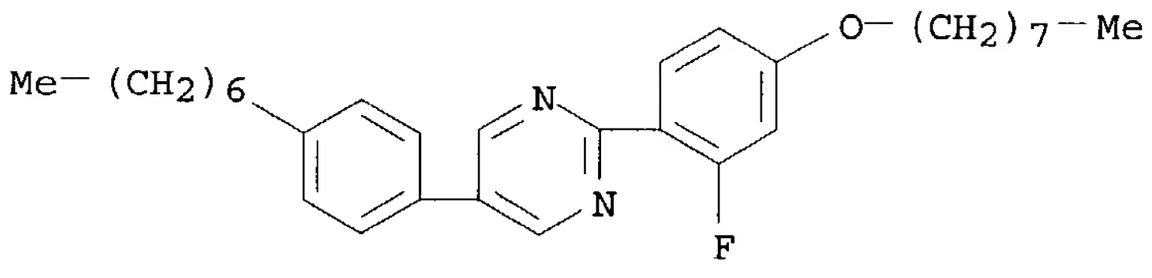
Absolute stereochemistry.



09/ 811,359

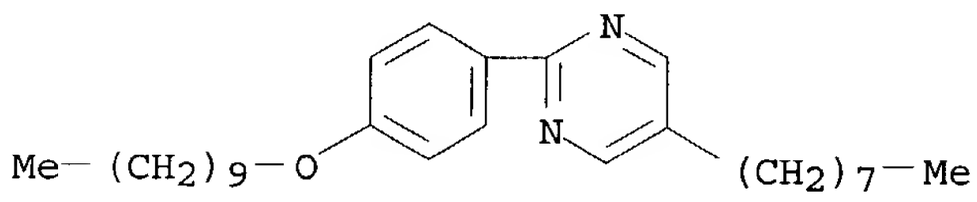
CM 2

CRN 124257-09-6
CMF C31 H41 F N2 O



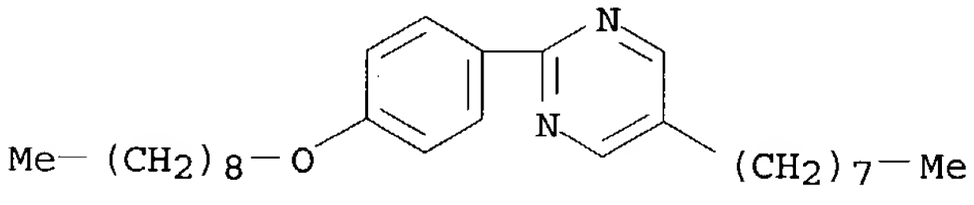
CM 3

CRN 57202-52-5
CMF C28 H44 N2 O



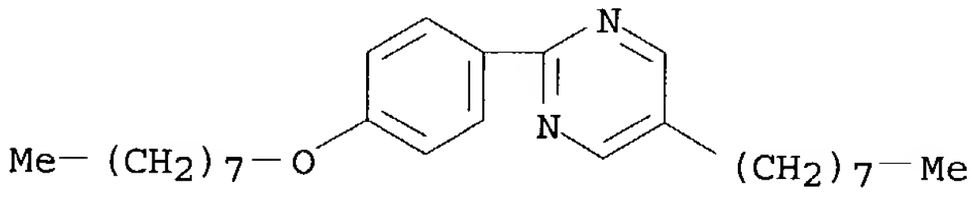
CM 4

CRN 57202-51-4
CMF C27 H42 N2 O



CM 5

CRN 57202-50-3
CMF C26 H40 N2 O



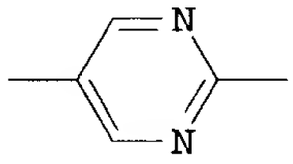
L11 ANSWER 59 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:14113 CAPLUS
DOCUMENT NUMBER: 118:14113
TITLE: Ferroelectric liquid crystal composition
INVENTOR(S): Saito, Goro; Yoshio, Kunikyo; Sato, Masahiro; Watanabe, Tetsuya

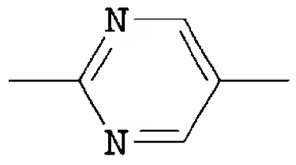
09/ 811,359

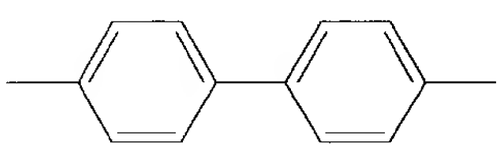
PATENT ASSIGNEE(S): NEC Corp., Japan; Sanyo Chemical Industries Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

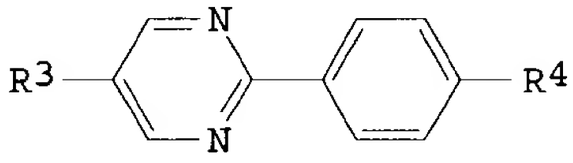
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 04126793 | A2 | 19920427 | JP 1990-249176 | 19900919 |

PRIORITY APPLN. INFO.: JP 1990-249176 19900919
GI


I


II

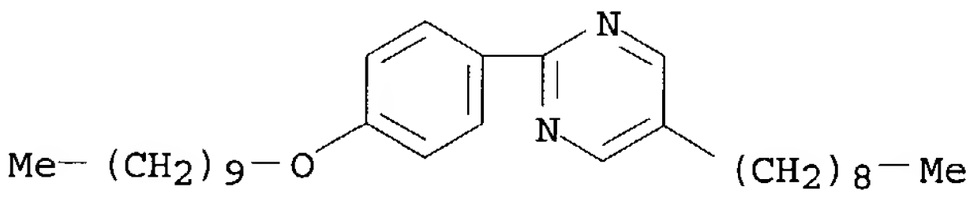

III


IV

AB The title liquid-crystal composition comprises ≥1 R1(XA)nYD(CH2)mC(CN)HR2 [R1,2 = C1-20 alkyl; X = O, single bond; Y = single bond, O, CO2, OCO, CH2O, OCH2, C.tplbond.C, CH2CH2; A = p-C6H4, I, II, III, 2,6-**naphthyl**; D = 2,6-**naphthyl**; n = 0,1] and ≥1 IV [R3,4 = C1-15 alkyl or alkoxy].

IT **144806-56-4**
RL: USES (Uses)
(ferroelec. liquid-crystal composition containing)

RN 144806-56-4 CAPLUS
CN Pyrimidine, 2-[4-(decyloxy)phenyl]-5-nonyl- (9CI) (CA INDEX NAME)



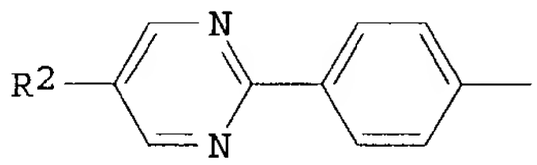
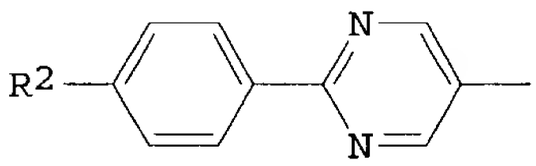

L11 ANSWER 60 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:612517 CAPLUS
DOCUMENT NUMBER: 117:212517
TITLE: Preparation of optically active 2-phenylpyrimidine derivatives, liquid crystal compositions containing them, and liquid crystal electrooptical devices
INVENTOR(S): Mihashi, Shigeru; Matsushima, Yoshimasa; Imai, Takashi; Mori, Kiichi; Yamada, Mamoru; Sugiyama, Hiroshi; Yagi, Misao; Kondo, Hitoshi; Hagiwara, Toshimitsu
PATENT ASSIGNEE(S): Takasago Perfumery Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 58 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 04154769 | A2 | 19920527 | JP 1990-279079 | 19901019 |
| JP 2627679 | B2 | 19970709 | | |
| US 6093345 | A | 20000725 | US 1993-91406 | 19930714 |

PRIORITY APPLN. INFO.: JP 1990-279079 A 19901019
US 1991-779528 B1 19911018

OTHER SOURCE(S): MARPAT 117:212517

GI

Q=  Q1= 

AB Optically active AO(CH2)nC*HF(CH2)mC*HXR1 (I; C* = asym. C atom; R1 = linear C2-5 alkyl; n = 1, 2; m = 0-3; X = F, Me; A = Q, Q1; R2 = linear C8-12 alkyl), useful as chiral dopants for nematic liquid crystals, are prepared A liquid crystal composition contains at least one I and a liquid crystal electrooptical device is obtained by injecting the latter composition Thus, 2-(4-hydroxyphenyl)-5-decylpyrimidine 3.0, (2R,5S)-2-tetrahydropyranyloxy-5-methylheptyl p-toluenesulfonate (preparation given) 6.0, K2CO3 2.1 g and 75 mL DMF were stirred for 18 h to give 77.5% (2'R,5'S)-2-[4-(2'-tetrahydropyranyloxy-5-methylheptyloxy)**phenyl**]-5-decylpyrimidine which was deprotected by p-toluenesulfonic acid in MeOH to give 68.2% an alc. and then fluorinated by hexafluoropropene-Et2NH adduct in CH2Cl2 to give 46.5% (2'S,5'S)-2-[4-(2'-fluoro-5'-methylheptyloxy)**phenyl**]-5-decylpyrimidine (II). II showed SC*-SA phase transition temperature 42.0° and a liquid crystal composition containing 9.3 mol% showed spontaneous polarization 3.1 nC/cm2, tilt angle 14°, and response speed 46 μs at TC-5°.

IT **144115-31-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(liquid crystal composition, for display device)

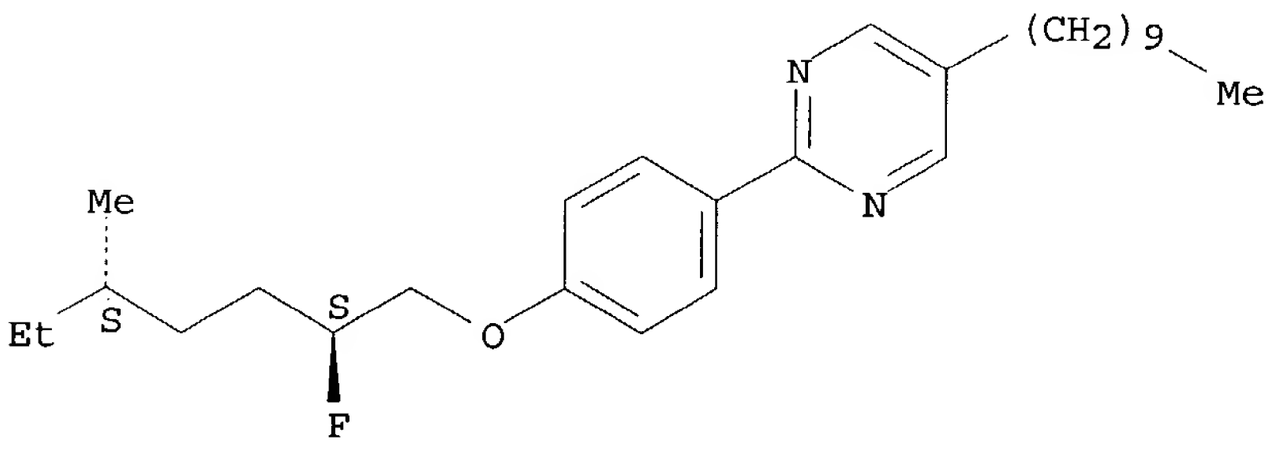
RN 144115-31-1 CAPLUS

CN Pyrimidine, 5-decyl-2-[4-[(2-fluoro-5-methylheptyl)oxy]phenyl]-, [S-(R*,R*)]-, mixt. with 2-[4-(decyloxy)phenyl]-5-octylpyrimidine, 5-heptyl-2-[4-(nonyloxy)phenyl]pyrimidine, 5-hexyl-2-[4-(octyloxy)phenyl]pyrimidine, 2-[4-(hexyloxy)phenyl]-5-octylpyrimidine and 5-octyl-2-[4-(octyloxy)phenyl]pyrimidine (9CI) (CA INDEX NAME)

CM 1

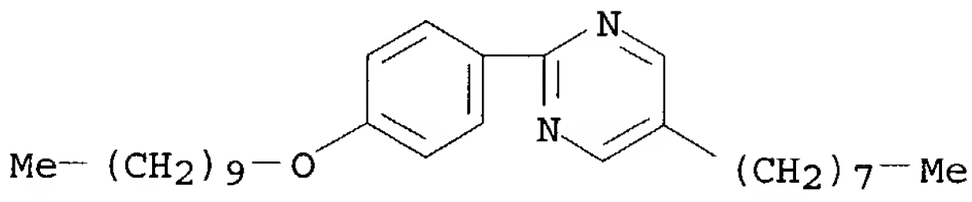
CRN 144088-30-2
CMF C28 H43 F N2 O

Absolute stereochemistry.



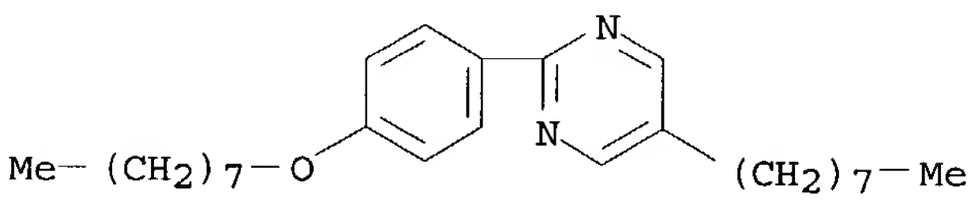
CM 2

CRN 57202-52-5
CMF C28 H44 N2 O



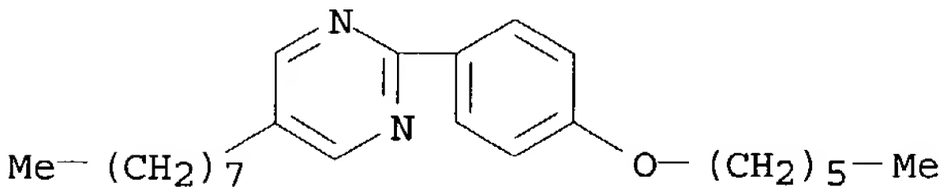
CM 3

CRN 57202-50-3
CMF C26 H40 N2 O



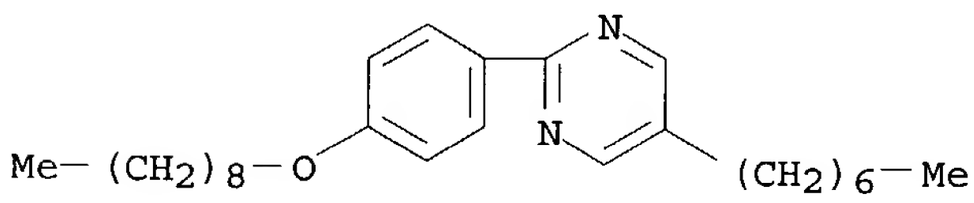
CM 4

CRN 57202-48-9
CMF C24 H36 N2 O



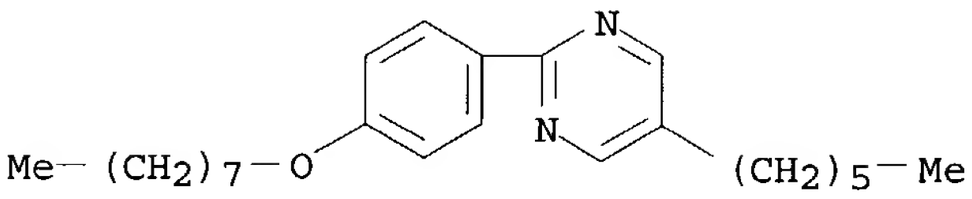
CM 5

CRN 57202-40-1
CMF C26 H40 N2 O



CM 6

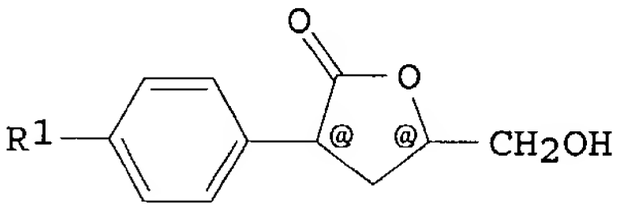
CRN 57202-30-9
CMF C24 H36 N2 O



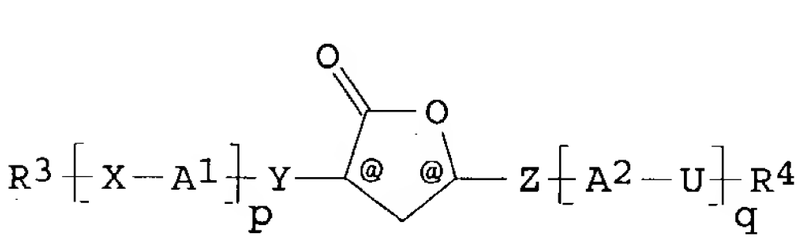
L11 ANSWER 61 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:83522 CAPLUS
DOCUMENT NUMBER: 116:83522
TITLE: Optically active **phenyl**(hydroxymethyl)-γ-butyrolactones and liquid crystal compositions containing them
INVENTOR(S): Sakashita, Keiichi; Hayashi, Shoji; Kamimura, Shigeo; Mori, Kenji
PATENT ASSIGNEE(S): Mitsubishi Rayon Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 03173879 | A2 | 19910729 | JP 1990-189223 | 19900717 |

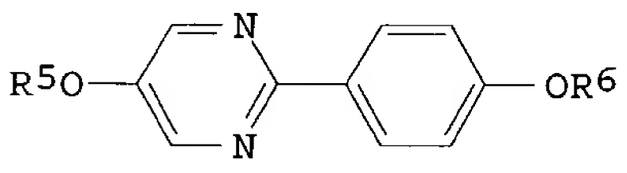
PRIORITY APPLN. INFO.: JP 1989-185769 19890718
OTHER SOURCE(S): MARPAT 116:83522
GI



I



II



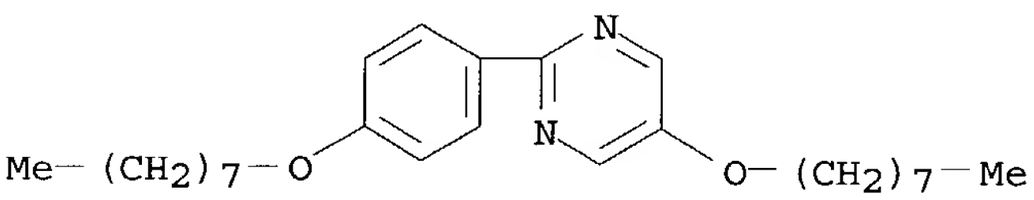
III

AB The title compds. [I; II; R1 = OH, CO2H, HOCH2, alkyl, alkoxy; R3, R4 = alkyl, alkenyl, alkynyl, alkoxyalkyl, alkylthioalkyl, etc.; X, U = O, CO2, O2C; Y, Z = single bond, O, CO2, O2C, CH2O, OCH2, A1, A2 = (substituted) phenylene, heteracyclohexylene, etc.; p, q = 0, 1; asterisk indicates chiral center] are prepared for liquid crystal compns. A solution of (S,S)-2-hydroxy-4-(butoxymethyl)-γ-butyrolactone, 4-[4-(undecanoyloxy)phenoxymethyl]benzoic acid, PPh3, and di-Et azodicarboxylate in benzene was allowed to react at room temperature overnight to give the corresponding title ester. A liquid crystal composition containing this and phenylpyrimidines III [R5 = C8H17, R6 = C6H13, C8H17, C12H25, C11H23; R5 = C6H13, R6 = C10H21, C9H19, C8H17] had transition temps. of -10, 62,

72 and 77° between crystalline and chiral smectic C phases, chiral smectic C and smectic A phases, smectic A and Ch phases, and Ch and Iso phases whereas a composition containing only III had transition temps. of 1, 63, 78, and 81°, resp.

IT **114767-84-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(liquid crystal compns. containing)

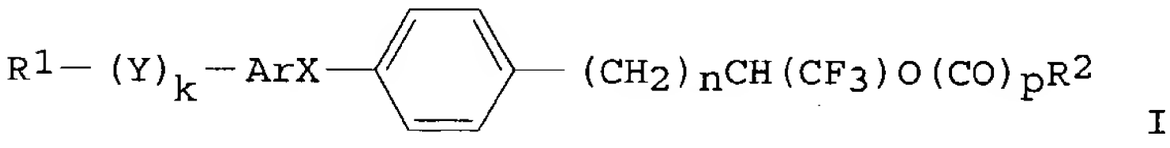
RN 114767-84-9 CAPLUS
CN Pyrimidine, 5-(octyloxy)-2-[4-(octyloxy)phenyl]- (9CI) (CA INDEX NAME)



L11 ANSWER 62 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:667057 CAPLUS
DOCUMENT NUMBER: 115:267057
TITLE: Preparation of optically active (aryl)trifluoromethylalkyl alkanoates and ethers for liquid-crystal compositions
INVENTOR(S): Kurimoto, Isao; Higashii, Takayuki; Toda, Shoji; Minai, Masayoshi; Sekine, Chizu; Tani, Takeshi; Fujisawa, Koichi
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 90 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| EP 434297 | A2 | 19910626 | EP 1990-313537 | 19901212 |
| EP 434297 | A3 | 19911106 | | |
| EP 434297 | B1 | 19961016 | | |
| R: CH, DE, FR, GB, LI | | | | |
| JP 03294246 | A2 | 19911225 | JP 1990-231539 | 19900829 |
| JP 2864698 | B2 | 19990303 | | |
| US 5238598 | A | 19930824 | US 1990-626980 | 19901213 |

PRIORITY APPLN. INFO.: JP 1989-329085 19891218
JP 1990-231539 19900829
JP 1989-234381 19890908
OTHER SOURCE(S): MARPAT 115:267057
GI



I

AB Optically active title compds. I [R1 = C3-26 alkyl; R2 = (halo) C1-20 alkyl or alkoxyalkyl; Ar = 1,4-phenylene, 4,4'-biphenylene, etc.; X = COO when n = 0 and COO or OCO when n = 1-5; Y = O, COO, OCO; k = 0,1; n = 0-5; p = 0, 1], useful for liquid crystal compns., were prepared Thus, 4-benzyloxy-α,α,α-trifluoroacetylphenone (preparation given)

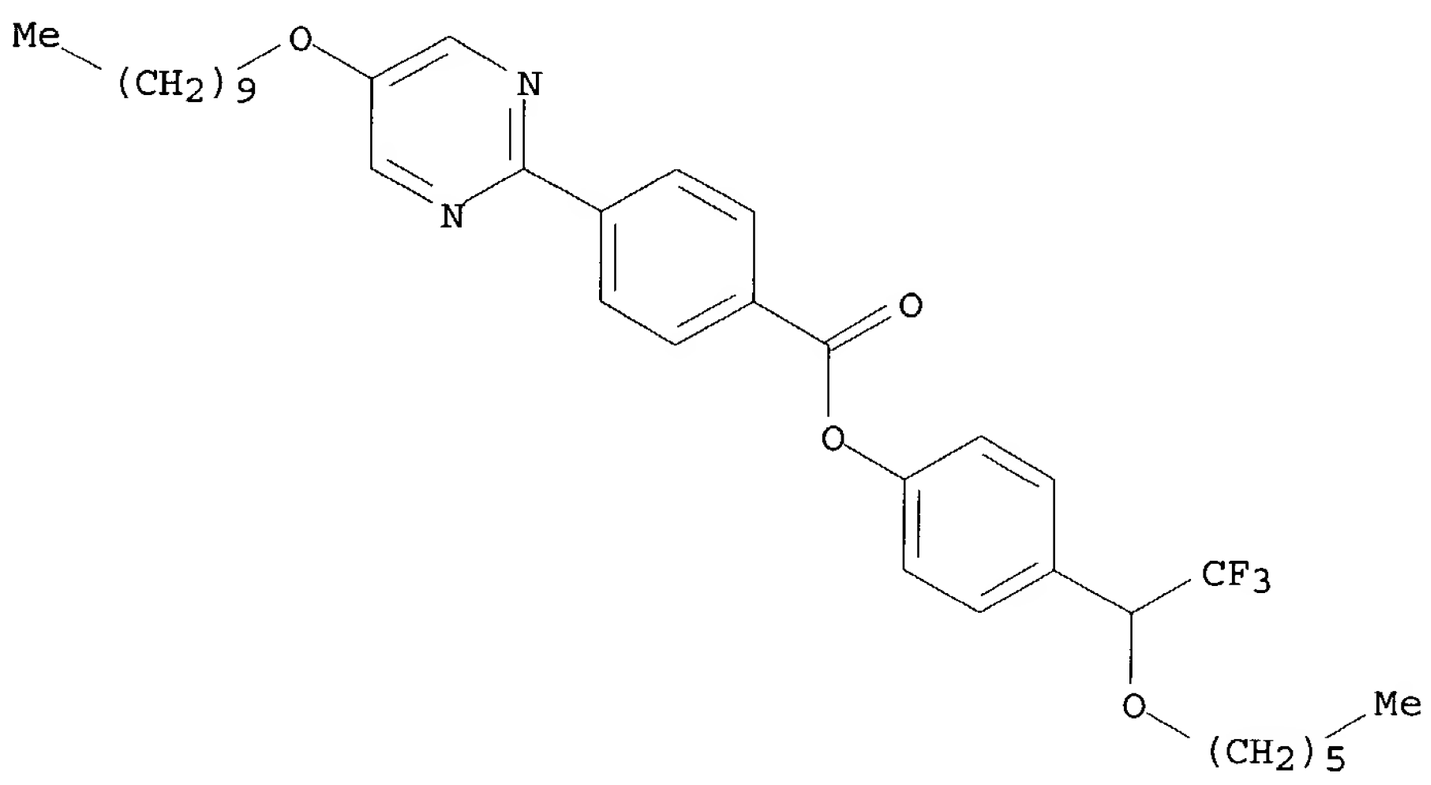
was subjected to NaBH4 reduction, acetylation of the alc. formed, and asym. hydrolysis to give (+)-4-benzyloxy-1-(1-acetoxy-2,2,2-trifluoroethyl)benzene. Alkylation by n-hexyl tosylate followed by debenzylation gave (+)-4-(1-hexyloxy-2,2,2-trifluoroethyl)phenol. This was stirred at room temperature for 24 h with 4-decyloxybenzene acid, DCC and anhydrous CH2Cl2 to give (+)-4-(1-hexyloxy-2,2,2-trifluoroethyl) **phenyl** 4-decyloxybenzoate (II). A liquid-crystal composition containing 20% II gave spontaneous polarization of -13 nC/cm2 at 20°.

IT **137614-98-3P**
RL: PREP (Preparation)
(preparation of, for liquid-crystal electrooptical display devices)

RN 137614-98-3 CAPLUS

CN Benzoic acid, 4-[5-(decyloxy)-2-pyrimidinyl]-, 4-[2,2,2-trifluoro-1-(hexyloxy)ethyl]phenyl ester, (+)- (9CI) (CA INDEX NAME)

Rotation (+).




L11 ANSWER 63 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:581603 CAPLUS
DOCUMENT NUMBER: 113:181603
TITLE: Optically-active 2-[4-(6-chloro-4-methylalkoxy) **phenyl**]-5-alkoxypyrimidines as chiral smectic liquid crystals
INVENTOR(S): Shibata, Toshihiro; Kimura, Masaki
PATENT ASSIGNEE(S): Adeka Argus Chemical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 02117667 | A2 | 19900502 | JP 1988-271752 | 19881027 |

PRIORITY APPLN. INFO.: JP 1988-271752 19881027

GI For diagram(s), see printed CA Issue.

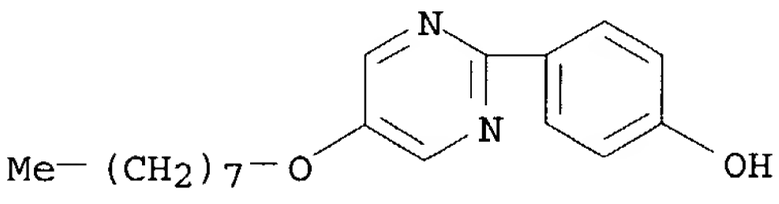
AB The title compds. I (R = C1-18 n-alkyl; R1 = H, C1-11 alkyl) are claimed. I show a chiral smectic phase at lower mesomorphic range than similar phenylpyrimidine derivs. in which 6-chloro-4-methylalkoxy are substituted with 4-methylhexyloxy, thus ferroelec. liquid-crystal compns. containing I are useful for electrooptical devices, such as liquid-crystal display. (+)-EtCHClCH2CHMe(CH2)3OH was treated with 2-(4-hydroxyphenyl)-5-

octyloxypyrimidine to give I (R = octyl, R1 = Et) (II), showing a chiral smectic C phase. A liquid-crystal display cell packed with II was prepared

IT **104539-91-5**, 2-(4-Hydroxyphenyl)-5-octyloxypyrimidine
RL: RCT (Reactant); RACT (Reactant or reagent)
(etherification of, with optically-active chloromethyloctanol, chiral smectic C liquid crystal from)

RN 104539-91-5 CAPLUS

CN Phenol, 4-[5-(octyloxy)-2-pyrimidinyl]- (9CI) (CA INDEX NAME)




L11 ANSWER 64 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:524525 CAPLUS
DOCUMENT NUMBER: 113:124525
TITLE: Optically active esters of 5-ethyl- and 5-vinyl-1,3-dioxolan-4-carboxylic acid, their preparation, their use as dopants in liquid-crystal mixtures, and liquid-crystal mixtures and display devices containing them
INVENTOR(S): Mueller, Ingrid; Duebal, Hans Rolf; Escher, Klaus; Hemmerling, Wolfgang; Illian, Gerhard; Murakami, Mikio; Ohlendorf, Dieter; Wingen, Rainer
PATENT ASSIGNEE(S): Hoechst A.-G., Germany
SOURCE: Ger. Offen., 13 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 3832503 | A1 | 19900329 | DE 1988-3832503 | 19880924 |
| EP 361272 | A1 | 19900404 | EP 1989-117265 | 19890919 |
| EP 361272 | B1 | 19940601 | | |
| R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE | | | | |
| AT 106402 | E | 19940615 | AT 1989-117265 | 19890919 |
| NO 8903778 | A | 19900326 | NO 1989-3778 | 19890922 |
| JP 02129179 | A2 | 19900517 | JP 1989-245378 | 19890922 |
| US 5328638 | A | 19940712 | US 1992-881520 | 19920512 |

PRIORITY APPLN. INFO.: DE 1988-3832503 19880924
EP 1989-117265 19890919
US 1989-410949 19890922

OTHER SOURCE(S): CASREACT 113:124525; MARPAT 113:124525

AB Tilted smectic liquid-crystal phases containing compds. of the invention as dopants had spontaneous polarization 50-100% higher than when they were doped with known compds. (4R,5R)-4-(5-n-Octylpyrimidin-2-yl) **phenyl** 2,2-dimethyl-5-vinyl-1,3-dioxolan-4-carboxylate was prepared from 4-(5-n-octylpyrimidin-2-yl)phenol and 2,2-dimethyl-5-vinyl-1,3-dioxolan-4-carboxylic acid.

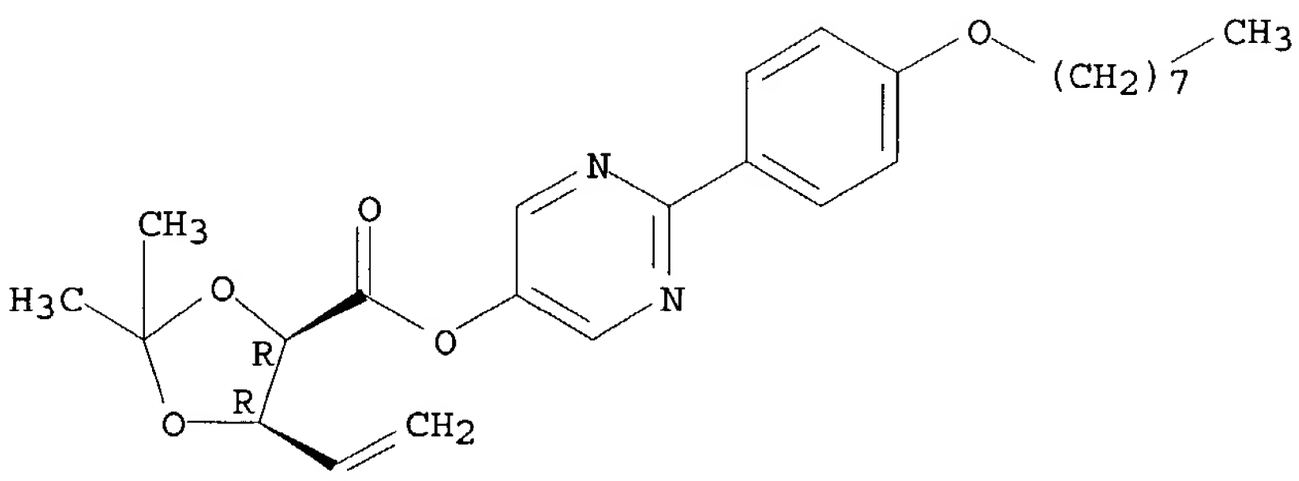
IT **129293-92-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as dopant for liquid-crystal mixture)

RN 129293-92-1 CAPLUS

CN 1,3-Dioxolane-4-carboxylic acid, 5-ethenyl-2,2-dimethyl-, 2-[4-(octyloxy)phenyl]-5-pyrimidinyl ester, (4R-cis)- (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

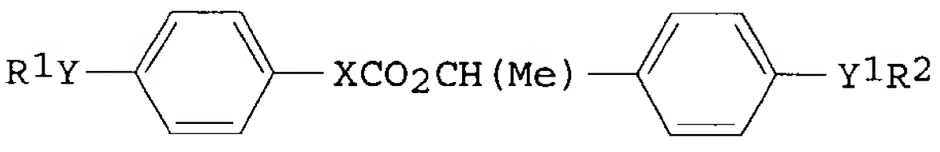


L11 ANSWER 65 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:227426 CAPLUS
DOCUMENT NUMBER: 112:227426
TITLE: α-(4-Substituted- **phenyl**)ethyl alcohol derivatives and liquid-crystal compositions containing them
INVENTOR(S): Koden, Mitsuhiro; Kuratate, Tomoaki; Funada, Fumiaki
PATENT ASSIGNEE(S): Sharp Corp., Japan
SOURCE: Ger. Offen., 15 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 3907507 | A1 | 19890921 | DE 1989-3907507 | 19890308 |
| DE 3907507 | C2 | 19900823 | | |
| JP 02019345 | A2 | 19900123 | JP 1988-169951 | 19880706 |
| JP 02036152 | A2 | 19900206 | JP 1988-183924 | 19880722 |
| JP 02040342 | A2 | 19900209 | JP 1988-191165 | 19880729 |
| JP 01316348 | A2 | 19891221 | JP 1988-332349 | 19881229 |
| JP 05088698 | B4 | 19931224 | | |
| GB 2216371 | A1 | 19891011 | GB 1989-5403 | 19890309 |
| GB 2216371 | B2 | 19920708 | | |
| US 5209867 | A | 19930511 | US 1991-815580 | 19911230 |

PRIORITY APPLN. INFO.:
JP 1988-57295 19880310
JP 1988-169951 19880706
JP 1988-183924 19880722
JP 1988-191165 19880729
US 1989-321079 19890309
US 1991-701346 19910505

GI



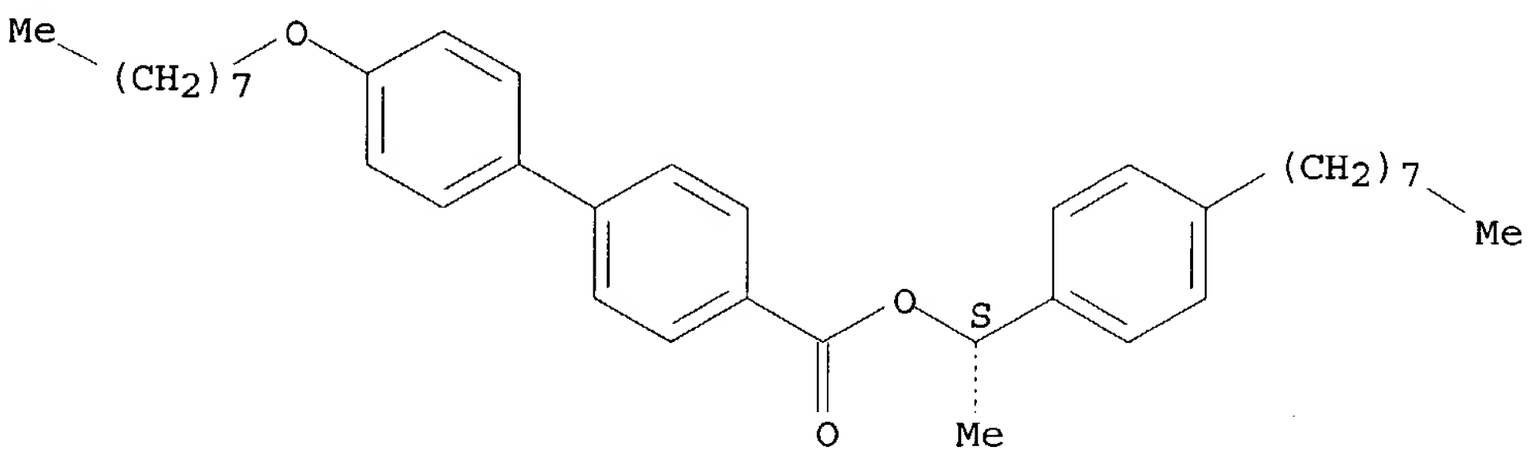
I

AB The title derivs. have the general formula I, where R1, R2 = C1-12 linear or branched alkyl; X = a single bond, 1,4-phenylene, or CH2; and Y, Y1 = a single bond or O.

IT **126130-05-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for smectic C liquid-crystal mixts.)
RN 126130-05-0 CAPLUS
CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-hexyl-, 4-(hexyloxy)phenyl ester, mixt. with 2-(4-butoxyphenyl)-5-hexylpyrimidine, 4-(hexyloxy)phenyl 4-(octyloxy)benzoate, 2-[4-(2-methylbutoxy)phenyl]-5-(undecyloxy)pyrimidine, 2-[4-[(4-methylhexyl)oxy]phenyl]-5-octylpyrimidine, 2-[4-[(6-methyloctyl)oxy]phenyl]-5-octylpyrimidine, 2-[4-[(3-methylpentyl)oxy]phenyl]-5-octylpyrimidine, 2-[4-[(3-methylpentyl)oxy]phenyl]-5-(undecyloxy)pyrimidine and 1-(4-octylphenyl)ethyl 4'-(octyloxy)[1,1'-biphenyl]-4-carboxylate (9CI) (CA INDEX NAME)

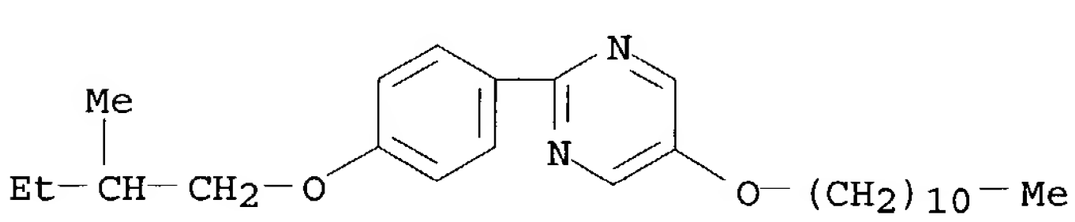
CM 1
CRN 126050-34-8
CMF C37 H50 O3

Absolute stereochemistry.



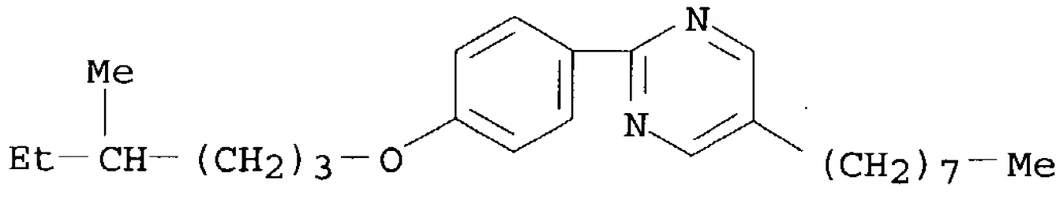

CM 2

CRN 118994-47-1
CMF C26 H40 N2 O2



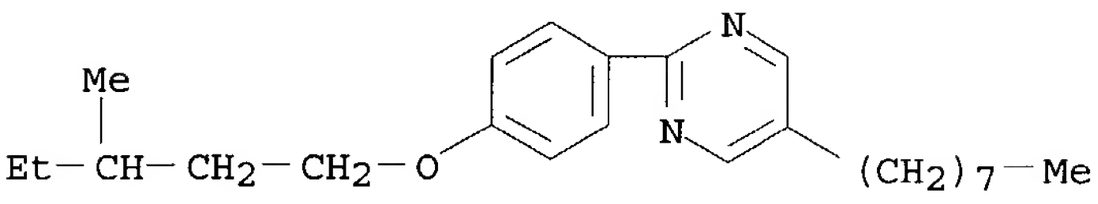

CM 3

CRN 116020-57-6
CMF C25 H38 N2 O



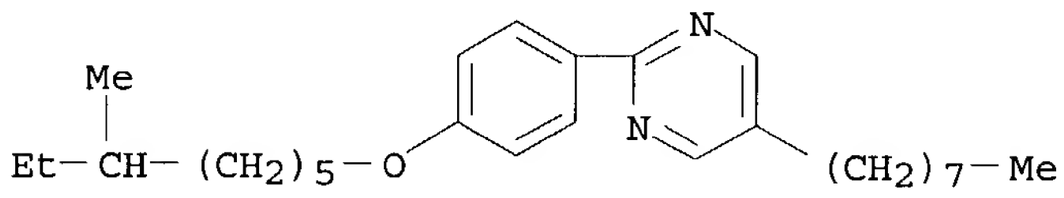

CM 4

CRN 116020-50-9
CMF C24 H36 N2 O



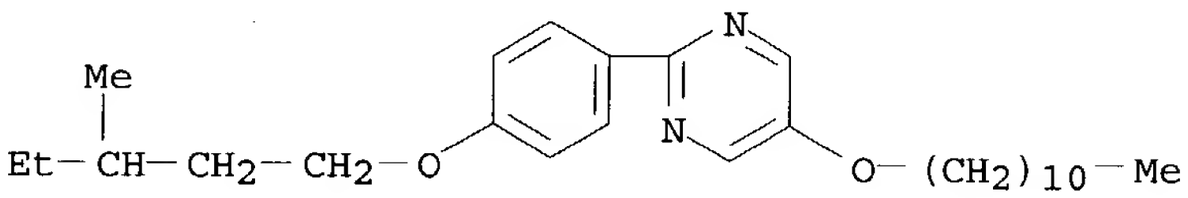
CM 5

CRN 108572-57-2
CMF C27 H42 N2 O



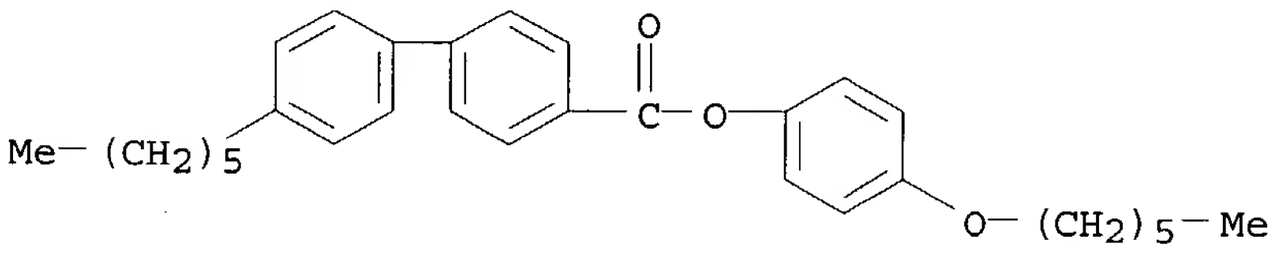
CM 6

CRN 108572-55-0
CMF C27 H42 N2 O2



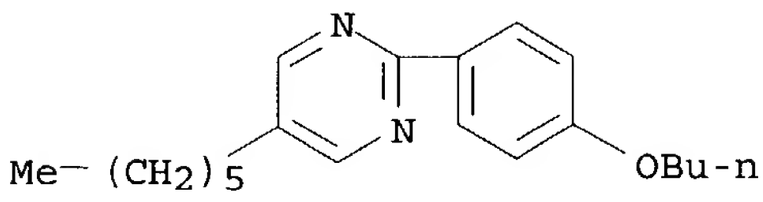
CM 7

CRN 62268-66-0
CMF C31 H38 O3



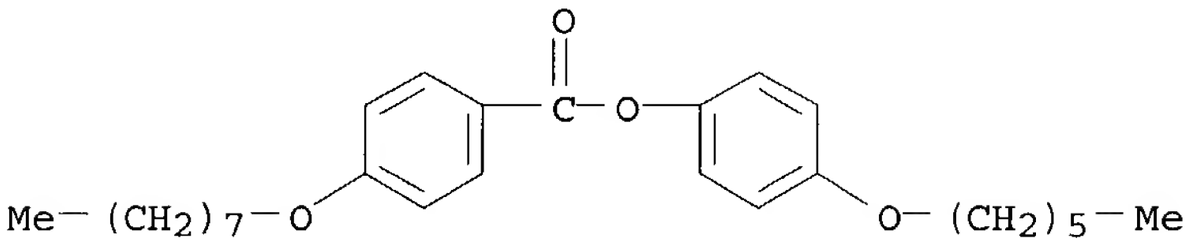
CM 8

CRN 57202-27-4
CMF C20 H28 N2 O



CM 9

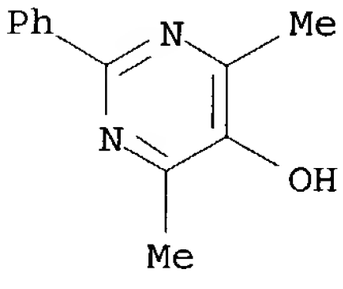
CRN 54963-63-2
CMF C27 H38 O4



L11 ANSWER 66 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:210534 CAPLUS
DOCUMENT NUMBER: 112:210534
TITLE: Chemiluminescent determination of antiradical activity of chemicals. II. 5-Hydroxypyrimidines
AUTHOR(S): Zolotov, N. N.; Zalilov, K. Yu.; Mukhtarov, V. E.; Gashev, S. B.; Smirnov, L. D.; Dyumaev, K. M.
CORPORATE SOURCE: NII Farmakol., Moscow, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1990), 24(1), 15-17
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB The antiradical activity of several alkyl and aryl derivs. of 5-hydroxypyrimidine was measured in a chemiluminescence system containing 3-hydroxypyridine, H2O2, and horseradish peroxidase. The results were compared with the data on luminescence quenching and lipophilicity of the agents determined by liquid chromatog. The structure-activity relationships are discussed. The results also correlated with reported data on cyclic nucleotide phosphodiesterase inhibition by the derivs. An immunostimulating activity of the compds. is suggested.

IT **75078-30-7**, 2-**Phenyl**-4,6-dimethyl-5-hydroxypyrimidine
RL: PRP (Properties)
(antioxidant effects of, lipophilicity and structure in relation to)
RN 75078-30-7 CAPLUS
CN 5-Pyrimidinol, 4,6-dimethyl-2-phenyl- (6CI, 9CI) (CA INDEX NAME)



L11 ANSWER 67 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:85747 CAPLUS

09/ 811,359

DOCUMENT NUMBER: 110:85747
TITLE: Use of optically active 1,3-dioxolan-4 carboxylic acid esters as dopants in liquid-crystal mixtures new optically active esters, and liquid-crystal mixtures and electrooptical devices containing them
INVENTOR(S): Wingen, Rainer; Duebal, Hans Rolf; Escher, Claus; Hemmerling, Wolfgang; Mueller, Ingrid; Ohlendorf, Dieter
PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 9 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 3713273 | A1 | 19881103 | DE 1987-3713273 | 19870418 |
| EP 288813 | A1 | 19881102 | EP 1988-105777 | 19880412 |
| EP 288813 | B1 | 19901114 | | |
| R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE | | | | |
| AT 58394 | E | 19901115 | AT 1988-105777 | 19880412 |
| NO 8801659 | A | 19881019 | NO 1988-1659 | 19880415 |
| NO 170885 | B | 19920914 | | |
| NO 170885 | C | 19921223 | | |
| CA 1339994 | A1 | 19980811 | CA 1988-564256 | 19880415 |
| JP 63304088 | A2 | 19881212 | JP 1988-92682 | 19880416 |
| JP 07017908 | B4 | 19950301 | | |
| US 5641428 | A | 19970624 | US 1992-879147 | 19920430 |

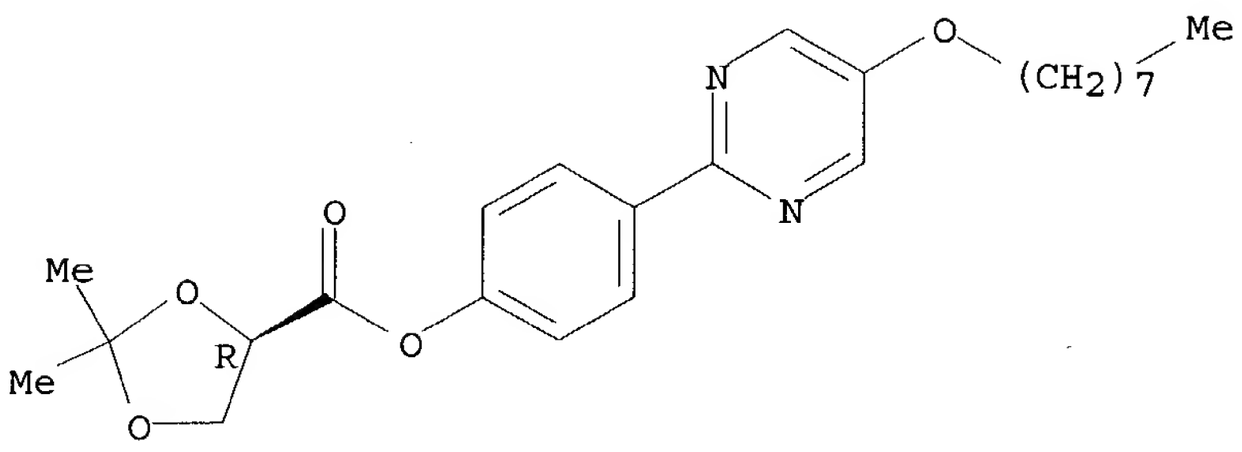
PRIORITY APPLN. INFO.: DE 1987-3713273 19870418
EP 1988-105777 19880412
US 1988-181925 19880415
US 1990-494909 19900309

OTHER SOURCE(S): CASREACT 110:85747

AB The optically active 1,3-dioxolan-4-carboxylic acid esters lead to ferroelec. liquid-crystal phases with short switching times and to electroclinic phases with large electroclinic coeffs. Their special advantage is that they induce a helix with a very large pitch, so that helix compensation by further dopants is unnecessary. These esters also have high UV stability. 4-(2-n-Octylpyrimidine-5-yl)phenol was reacted with 2,2-dimethyl-1,3-dioxolan-4-carboxylic acid chloride to form (R)-4-(2-n-octylpyrimidine-5-yl)**phenyl** 2,2-dimethyl-1,3-dioxolan-4-carboxylate, m. 88° and having optical rotation [α] D3 = +7.54.

IT **118808-39-2P**
RL: PREP (Preparation)
(preparation of, for liquid-crystal phases for electrooptical devices)
RN 118808-39-2 CAPLUS
CN 1,3-Dioxolane-4-carboxylic acid, 2,2-dimethyl-, 4-[5-(octyloxy)-2-pyrimidinyl]phenyl ester, (R)- (9CI) (CA INDEX NAME)

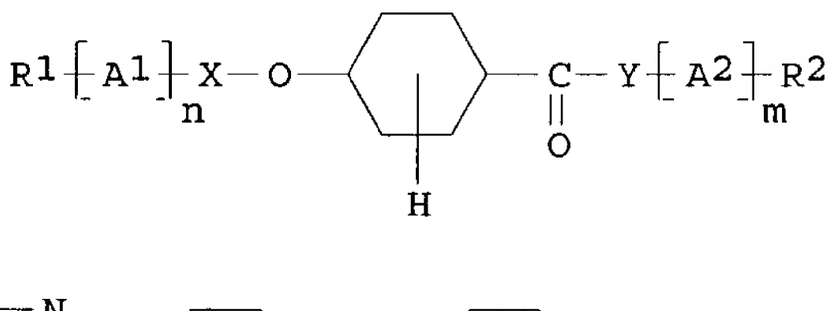
Absolute stereochemistry.



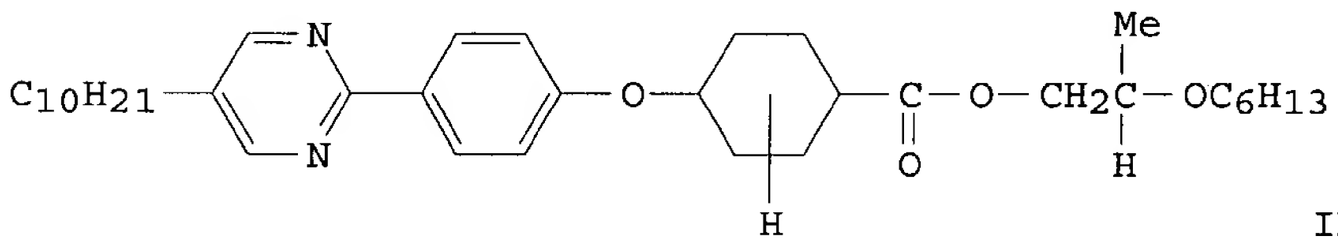
L11 ANSWER 68 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:15974 CAPLUS
DOCUMENT NUMBER: 110:15974
TITLE: Ferroelectric liquid-crystal display device
INVENTOR(S): Yamashita, Masataka; Yamada, Yoko; Kadokano, Goji; Hioki, Cheko; Iwaki, Takashi
PATENT ASSIGNEE(S): Canon K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 63137986 | A2 | 19880609 | JP 1986-283476 | 19861128 |

PRIORITY APPLN. INFO.: JP 1986-283476 19861128
GI



I



II

AB The title device uses I (R1, R2 = chain radical; A1, A2 = divalent radical containing six-membered ring(s); X, Y = bond or divalent chain radical; n, m = 0 .apprx. 1 with n + m = 1) in the liquid crystal layer. Thus, a mixture of II 10, 4'-(2-ethoxypropyloxy)**phenyl** p-decyloxybenzoate 50, and 4'-(4-methylhexyloxy)**phenyl** p-decyloxybenzoate 50 weight parts was sealed in a cell and cooled at 0.5°/h from its isotropic phase to 20°. The liquid crystal composition had 325 and 245 μs in response time at 10 and 30°, resp.

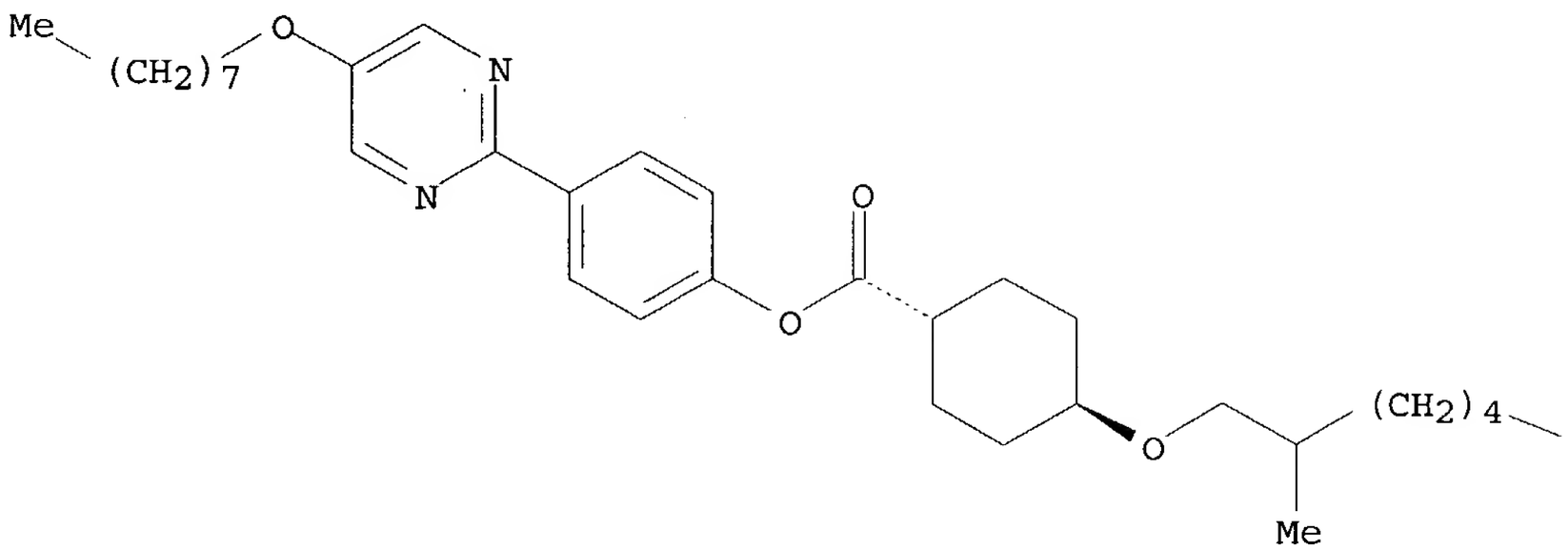
IT **117907-26-3**
RL: TEM (Technical or engineered material use); USES (Uses)
(liquid crystal compns. containing, for electrooptical display devices)

RN 117907-26-3 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[(2-methylheptyl)oxy]-, 4-[5-(octyloxy)-2-

pyrimidinyl]phenyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A




PAGE 1-B

L11 ANSWER 69 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:449772 CAPLUS
DOCUMENT NUMBER: 107:49772
TITLE: Smectic liquid-crystal phases
INVENTOR(S): Hopf, Reinhard; Scheuble, Bernhard; Waechtler, Andreas; Hittich, Reinhard; Eidenschink, Rudolf; Geelhaar, Thomas; Krause, Joachim; Reiffenrath, Volker
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Fed. Rep. Ger.
SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 8701717 | A2 | 19870326 | WO 1986-EP529 | 19860915 |
| WO 8701717 | A3 | 19870521 | | |
| W: JP, KR, NO, US | | | | |
| RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE | | | | |
| DE 3533333 | A1 | 19870326 | DE 1985-3533333 | 19850918 |
| DE 3608500 | A1 | 19870924 | DE 1986-3608500 | 19860314 |

| | | | | | |
|---|---|---|---|---|---|
| WO 8705618 | | A1 | 19870924 | WO 1986-EP513 | 19860905 |
| | W: JP, KR, US | | | | |
| | RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE | | | | |
| EP 259346 | | A1 | 19880316 | EP 1986-905771 | 19860905 |
| EP 259346 | | B1 | 19900404 | | |
| | R: CH, DE, FR, GB, LI, SE | | | | |
| JP 63502657 | | T2 | 19881006 | JP 1986-505063 | 19860905 |
| JP 63500948 | | T2 | 19880407 | JP 1986-504895 | 19860915 |
| JP 2777885 | | B2 | 19980723 | | |
| DD 249707 | | A5 | 19870916 | DD 1986-294526 | 19860918 |
| US 4886620 | | A | 19891212 | US 1987-51120 | 19870513 |
| NO 8702040 | | A | 19870515 | NO 1987-2040 | 19870515 |

PRIORITY APPLN. INFO.:

| | |
|---|---|
| DE 1985-3533333 | 19850918 |
| DE 1986-3608500 | 19860314 |
| WO 1986-EP513 | 19860905 |
| WO 1986-EP529 | 19860915 |

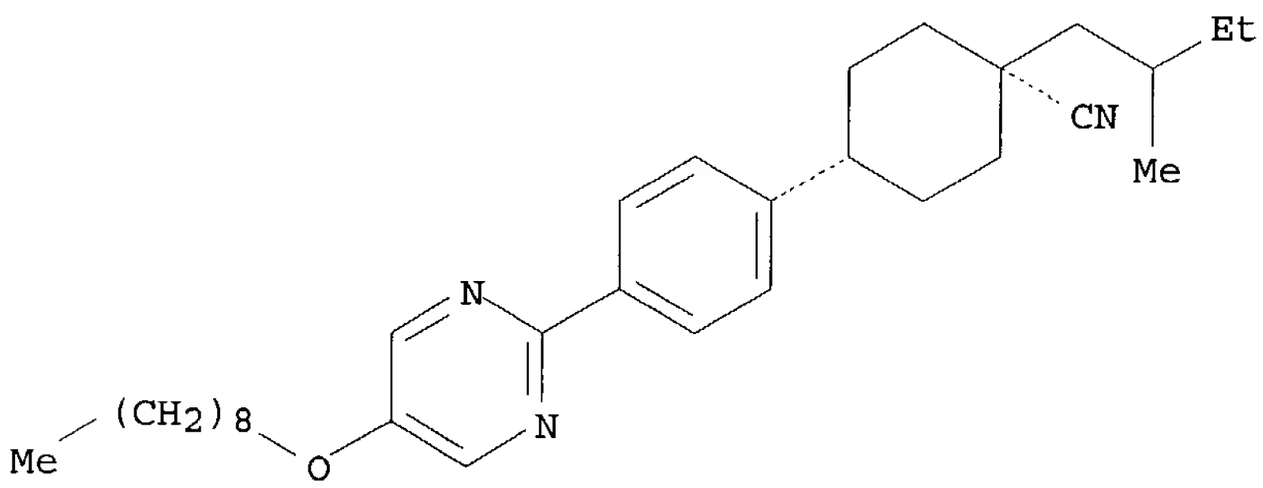
AB Compds. having neg. dielec. anisotropy for chiral smectic liquid-crystal phases used in electrooptical display devices are described. A liquid-crystal phase containing 4-(5-heptylpyrimidin-2-yl)**phenyl** (p-pentylbenzyl) ether 25, 4-(5-heptylpyrimidin-2-yl)**phenyl** (p-hexylbenzyl) ether 33, 4-(5-nonylpyrimidin-2-yl)**phenyl** (p-pentylbenzyl) ether 12, 4-(5-nonylpyrimidin-2-yl)**phenyl** (p-hexylbenzyl) ether 3, 2-p-nonyloxyphenyl-5-nonylpyrimidine 21, 2,3-dicyano-1,4-bis(trans-4-propylcyclohexylcarboxy)benzene 3, and 2,3-dicyano-1,4-bis(trans-4-pentylcyclohexylcarboxy)benzene 3% had crystalline-smectic C, smectic C-nematic, and nematic-isotropic phase transitions at 7, 64, and 95.5°, resp., and dielec. anisotropy -0.5.

IT **109203-83-0**
RL: USES (Uses)
(smectic liquid-crystal compns. containing, for display devices)

RN 109203-83-0 CAPLUS

CN Cyclohexanecarbonitrile, 1-(2-methylbutyl)-4-[4-[5-(nonyloxy)-2-pyrimidinyl]phenyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

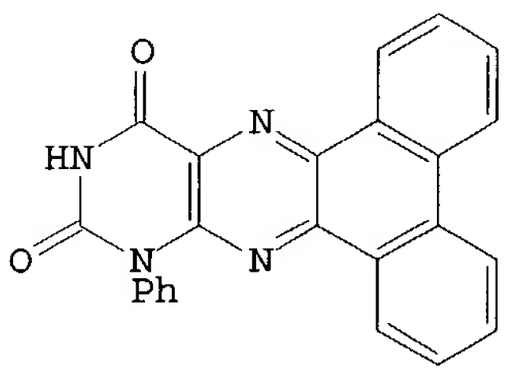



L11 ANSWER 70 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

| | |
|---|---|
| ACCESSION NUMBER: | 1981:443037 CAPLUS |
| DOCUMENT NUMBER: | 95:43037 |
| TITLE: | Synthesis of 2,4-substituted 6,7-phenanthreno- and 6,7-acenaphthenopteridines |
| AUTHOR(S): | Ram, Vishnu J.; Pandey, Hrishi Kesh; Vlietinck, Arnold J. |
| CORPORATE SOURCE: | Dep. Chem., S. C. Coll., Ballia, India |
| SOURCE: | Journal of Heterocyclic Chemistry (1981), 18, 55-7<br>CODEN: JHTCAD; ISSN: 0022-152X |
| DOCUMENT TYPE: | Journal |
| LANGUAGE: | English |

09/ 811,359

OTHER SOURCE(S): CASREACT 95:43037
GI

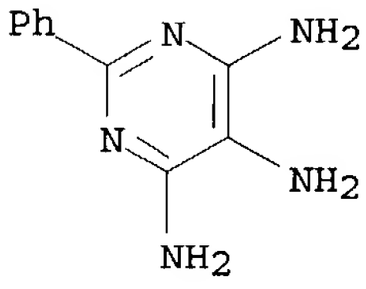


I

AB A series of 2- and 4-substituted 6,7-phenanthreno- and 6,7-acenaphthenopteridines were prepared The structures of the compds. were confirmed by spectroscopic studies and elemental analyses. Thus, 1-**phenyl**-2,4-dioxa-5,6-diaminopyridine was treated with phenanthroquinone to give the phenanthrenopyrimidopyrazine I.

IT **78270-90-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with phenanthraquinone and acenaphthone)

RN 78270-90-3 CAPLUS
CN 4,5,6-Pyrimidinetriamine, 2-phenyl- (9CI) (CA INDEX NAME)



L11 ANSWER 71 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:120945 CAPLUS
DOCUMENT NUMBER: 86:120945
TITLE: Synthesis and effect of some adamantane derivatives on the Sindbis virus
AUTHOR(S): Danilenko, G. I.; Vladimirtsev, I. F.; Yurchenko, A. G.; Galegov, G. A.; Leont'eva, N. O.; Isaev, S. D.; Dikolenko, E. I.; Boldyrev, I. V.; Yurchenko, R. I.; Kotenko, S. I.
CORPORATE SOURCE: Inst. Org. Chem., Kiev, USSR
SOURCE: Farmatsevtichnii Zhurnal (Kiev) (1976), (5), 36-40
CODEN: FRZKAP; ISSN: 0367-3057
DOCUMENT TYPE: Journal
LANGUAGE: Ukrainian
OTHER SOURCE(S): CASREACT 86:120945

AB 1-(4-Tolyl)- and 1-(4-anisyl)adamantane-3-carboxylic acids reacted with PCl5 in refluxing CCl4 and were treated with 25% aqueous NH3 to give the resp. amides, which were treated with NaOMe in MeOH and then with Br to give the corresponding 3-[(N-methoxycarbonyl)amino]adamantanes. Treating adamantane-1-carbonyl chloride with 9 amines (e.g., 2-, 3-, and 4-MeOC6H4NH2, piperidine, 4,6-dichloropyrimidine) afforded the resp. amides; those derived from primary and from Et2NH were active against Sindbis virus reproduction, as were 1-(N-methacryloylamino)adamantane and its copolymer with (diethylamino)ethyl N-methacryloylanthranilate-HCl. (Adamantoylmethylene)triphenylphosphorane cyclized with RN3 (R = Ph, 4-O2NC6H4) to give 72-83% 5-(1-adamantyl)-1-aryl-1,2,3-triazoles.

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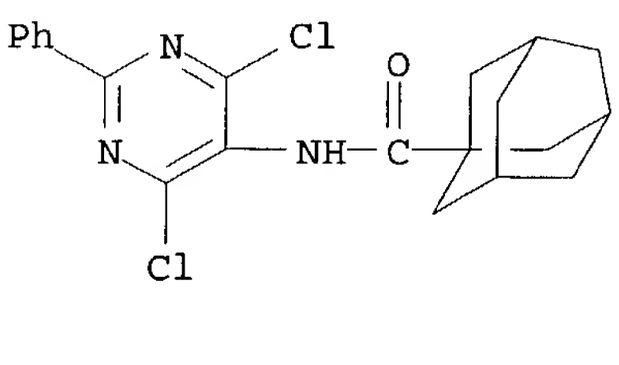
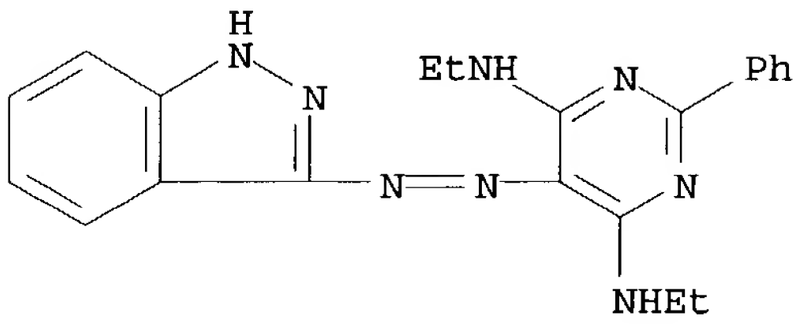
IT **62248-28-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and virucidal activity of)
RN 62248-28-6 CAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-carboxamide, N-(4,6-dichloro-2-phenyl-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



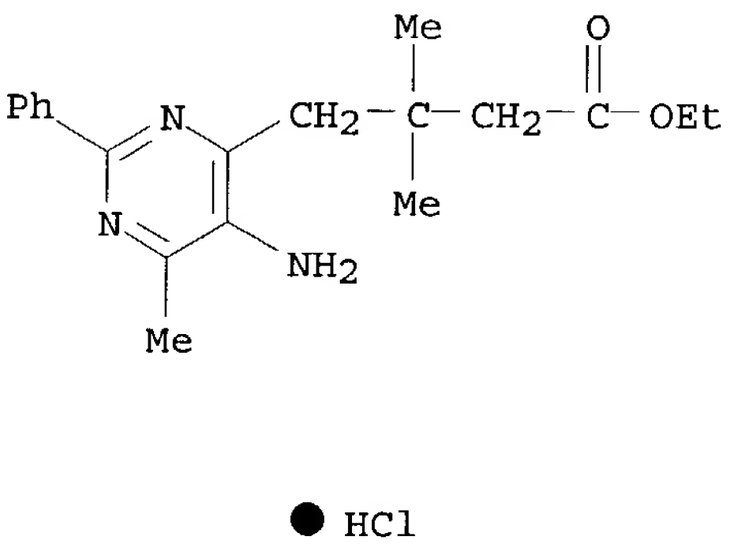

L11 ANSWER 72 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1976:107079 CAPLUS
DOCUMENT NUMBER: 84:107079
TITLE: Polycyclic dyes
INVENTOR(S): Dehnert, Johannes; Dunkelmann, Guenter
PATENT ASSIGNEE(S): BASF A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 26 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 2430565 | A1 | 19760115 | DE 1974-2430565 | 19740626 |
| DE 2430565 | B2 | 19771027 | | |
| GB 1504532 | A | 19780322 | GB 1975-21447 | 19750520 |
| CH 612212 | A | 19790713 | CH 1975-8141 | 19750623 |
| FR 2276358 | A1 | 19760123 | FR 1975-19708 | 19750624 |
| JP 51018735 | A2 | 19760214 | JP 1975-78684 | 19750626 |

PRIORITY APPLN. INFO.: DE 1974-2430565 19740626
GI For diagram(s), see printed CA Issue.
AB Seven polycyclic dyes (I, R = H, Cl; R1 = H, NO2; R2 = NH2, NHEt, NHCH2CH2OH, NMeCH2CH2OH, Me, NHCH2CH2CH2OMe, NHCH2CH2OCH2CH2OH; R3 = Ph, p-ClC6H4, NBu2, Me) were prepared and dyed polyester fibers fast, brilliant greenish yellow to yellow shades. Thus, 3-amino-6-chloroindazole [16889-21-7] was diazotized, coupled with 2-**phenyl**-4,6-diaminopyrimidine [52644-22-1] to give the azo derivative (II) [**58514-83-3**], and II heated in a boiling HOAc-H2SO4 mixture for 12 hr to give I (R = Cl, R1 = H, R2 = NH2, R3 = Ph) [58514-84-4]. The other I were similarly prepared
IT **58514-73-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)
RN 58514-73-1 CAPLUS
CN 4,6-Pyrimidinediamine, N,N'-diethyl-5-(1H-indazol-3-ylazo)-2-phenyl- (9CI) (CA INDEX NAME)



L11 ANSWER 73 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1973:526438 CAPLUS
DOCUMENT NUMBER: 79:126438
TITLE: 2-Oxo-4,4,9-trimethyl-7-**phenyl**-2,3,4,5-tetrahydro-(1H)-pyrimido[5,4-b] azepine
AUTHOR(S): Strakov, A. Ya.; Brutane, D.
CORPORATE SOURCE: Rizh. Politekh. Inst., Riga, USSR
SOURCE: Latvijas PSR Zinatnu Akademijas Vestis, Kimijas Serija (1973), (2), 225-9
CODEN: LZAKAM; ISSN: 0002-3248
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Pyrimidoazepinone (I) was prepared in 50% yield by heating quinazolone (II; X = O) with NaN3 in polyphosphoric acid and in 90% yield by heating tosyloxime (II; X = NOSO2C6H4Me-p) in AcOH with Beckmann rearrangement.
IT **50681-88-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 50681-88-4 CAPLUS
CN 4-Pyrimidinebutanoic acid, 5-amino-β,β,6-trimethyl-2-phenyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

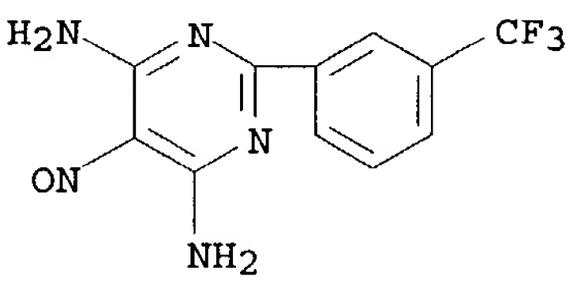


● HCl

L11 ANSWER 74 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1967:403074 CAPLUS
DOCUMENT NUMBER: 67:3074
TITLE: Pteridinecarboxamide diuretics. II. Reaction of 4,6-diamino-5-nitrosopyrimidines with N-substituted cyanoacetamides
AUTHOR(S): Osdene, Thomas S.; Santilli, Arthur A.; McCardle, Lee E.; Rosenthale, Marvin E.
CORPORATE SOURCE: Res. and Develop. Div., Wyeth Labs. Inc., Radnor, PA, USA
SOURCE: Journal of Medicinal Chemistry (1967), 10(2), 165-7
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal

09/ 811,359

LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB cf. CA 65: 12204g. Several new 4,6-diamino-2-substituted 5-nitrosopyrimidines and N-substituted 2-cyanoacetamides were prepared and used as intermediates in the base-catalyzed preparation of a number of 4,7-diamino-2-substituted N-substituted 6-pteridinecarboxamides as shown. Many of these pteridines had diuretic activity in rats after oral administration. Increased activity was associated with certain specific structural characteristics. The more active compds. were those in which the 2 position of the pteridine nucleus bears an aromatic group, preferably **phenyl** or m-chlorophenyl, and in which the carbamoyl N bears a 2-dialkylaminoethyl or 2-(N-heterocyclic amino)ethyl group, e.g., 2-diethylaminoethyl or 2-morpholinoethyl.
IT **15059-97-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 15059-97-9 CAPLUS
CN Pyrimidine, 4,6-diamino-5-nitroso-2-(α,α,α-trifluoro-m-tolyl)- (8CI) (CA INDEX NAME)




=> d his

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FILE 'REGISTRY' ENTERED AT 10:41:51 ON 21 FEB 2004
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L2 STRUCTURE UPLOADED
L3 STRUCTURE UPLOADED
L4 8401 S L1 FUL
L5 5166 S L2 FUL
L6 316 S L3 FUL

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L8 878 S L7 NOT (PYRIDYL OR PYRIDIN? OR PYRIMIDIN? OR PYRIMIDYL OR PYR
L9 81 S L8 AND (PHENYL OR NAPHTHYL)
L10 68 S L6
L11 74 S L9 NOT L10